National Library of Canada
Acquisitions and Bibliographic Services Branch
395 Wellington Street
Ottawa, Ontario
K1A 0N4

Bibliothèque nationale du Canada
Direction des acquisitions et des services bibliographiques
395, rue Wellington
Ottawa (Ontario)
K1A 0N4

Your file Votre référence

Our file Notre référence

NOTICE

The quality of this microform is heavily dependent upon the quality of the original thesis submitted for microfilming. Every effort has been made to ensure the highest quality of reproduction possible.

If pages are missing, contact the university which granted the degree.

Some pages may have indistinct print especially if the original pages were typed with a poor typewriter ribbon or if the university sent us an inferior photocopy.

Reproduction in full or in part of this microform is governed by the Canadian Copyright Act, R.S.C. 1970, c. C-30, and subsequent amendments.

AVIS

La qualité de cette microforme dépend grandement de la qualité de la thèse soumise au microfilmage. Nous avons tout fait pour assurer une qualité supérieure de reproduction.

S'il manque des pages, veuillez communiquer avec l'université qui a conféré le grade.

La qualité d'impression de certaines pages peut laisser à désirer, surtout si les pages originales ont été dactylographiées à l'aide d'un ruban usé ou si l'université nous a fait parvenir une photocopie de qualité inférieure.

La reproduction, même partielle, de cette microforme est soumise à la Loi canadienne sur le droit d'auteur, SRC 1970, c. C-30, et ses amendements subséquents.

Canada

UNIVERSITY OF ALBERTA

RADIATION TRANSPORT

BY

HUMAYON BUTT

A thesis submitted to the faculty of Graduate Studies and Research in partial fulfilment of the requirement for the degree of Master of Science.

IN

DEPARTMENT OF ELECTRICAL ENGINEERING

EDMONTON, ALBERTA

FALL 1993

National Library
of Canada

Acquisitions and
Bibliographic Services Branch

395 Wellington Street
Ottawa, Ontario
K1A 0N4

Bibliothèque nationale
du Canada

Direction des acquisitions et
des services bibliographiques

395, rue Wellington
Ottawa (Ontario)
K1A 0N4

Your file Votre référence

Our file Notre référence

The author has granted an irrevocable non-exclusive licence allowing the National Library of Canada to reproduce, loan, distribute or sell copies of his/her thesis by any means and in any form or format, making this thesis available to interested persons.

L'auteur a accordé une licence irrévocable et non exclusive permettant à la Bibliothèque nationale du Canada de reproduire, prêter, distribuer ou vendre des copies de sa thèse de quelque manière et sous quelque forme que ce soit pour mettre des exemplaires de cette thèse à la disposition des personnes intéressées.

The author retains ownership of the copyright in his/her thesis. Neither the thesis nor substantial extracts from it may be printed or otherwise reproduced without his/her permission.

L'auteur conserve la propriété du droit d'auteur qui protège sa thèse. Ni la thèse ni des extraits substantiels de celle-ci ne doivent être imprimés ou autrement reproduits sans son autorisation.

ISBN 0-315-88123-2

Canada

UNIVERSITY OF ALBERTA
RELEASE FORM

NAME OF AUTHOR:	**HUMAYON BUTT**
TITLE OF THESIS:	**RADIATION TRANSPORT FOR THE MEDUSA CODE**
DEGREE:	**MASTER OF SCIENCE**
FIELD OF STUDY:	**LASER PLASMA INTERACTION**
YEAR THIS DEGREE GRANTED:	**1993**

Permission is hereby granted to the University of Alberta Library to reproduce single copies of this thesis and to lend or sell such copies for private, scholarly or scientific research purposes only.

The author reserves all other publication and other rights in association with the copyright in the thesis and except as hereinbefore provided neither the thesis nor any substantial portion thereof may be printed or otherwise reproduce in any form without the author's prior written permission.

Humayon Butt

Apt 1909
11135 83 Ave
Edmonton, Alberta
T6G 2C6
Canada

MAy. 11 1993

UNIVERSITY OF ALBERTA

FACULTY OF GRADUATE STUDY

The undersigned certify that they have read and recommended to the faculty of Graduate Studies and Research for acceptance, a thesis entitled RADIATION TRANSPORT FOR THE MEDUSA CODE in partial fulfilment of the requirement for the degree of Master of Science in Laser Plasma interaction.

Dr. C. E. Capjack

Dr. C. R. James

Dr. R. Rankin

Dr. R. Fedosejves

Dr. J. C. Samson

Jan. 08 1993

TABLE OF CONTENTS

CHAPTER ONE: INTRODUCTION

1.1	Laser Driven Nuclear Fusion	02
1.2	Physics Of Laser Produced Plasma	03
1.3	Objective And Organization Of The Thesis	07

CHAPTER TWO: RADIATIVE TRANSFER EQUATION

2.1	Derivation Of The Radiative Transfer Equation	09
2.2	Validity Of The Radiative Transfer Equation	12

CHAPTER THREE: DIFFUSION SYNTHETIC ACCELERATION

3.1	Introduction	15
3.2	Brief History	15
3.3	Discretization Of The Radiative Transfer Equation	16
3.3.1	Discretization In Time	17
3.3.2	Discretization In Frequency	18
3.3.3	Discretization In Angular Space	19
3.3.4	Discretization In Space	20
3.4	Source Iteration (SI)	20
3.5	Synthetic Acceleration Of The Transfer Equation	21
3.5.1	Introduction To Synthetic Acceleration	21
3.5.2	Diffusion Synthetic Acceleration (DSA)	23
3.6	Grey Diffusion Equation	25

CHAPTER FOUR: MODEL PROBLEM

4.1	Fixups And The Stability Of The Code	29
4.2	Theoretical Aspects Of The Model Problem	32
4.3	Simulations Of The Model Problem	34

CHAPTER FIVE: MEDUSA SIMULATIONS:

5.1	Introduction To MEDUSA	51
5.1.1	Physical Model	52
5.1.2	Energy Equation	53
5.1.3	Heat Conduction	54
5.1.4	Energy Exchange	54
5.1.5	Energy Emitted	54
5.1.6	Energy Absorbed	54
5.1.7	Motion Of Plasma	55
5.1.8	Equation Of State	55
5.1.9	Differencing Schemes	55

5.1.10 Time Differencing And Time Step Control 56
5.1.11 Laser Profile 56
5.2 Integration Of The Radiation Code In MEDUSA 57
5.3 MEDUSA Simulations 61
5.4 Concluding Remarks 88

BIBLIOGRAPHY 90

APPENDIX:

A. NUMERICAL ASPECTS OF DSA
A.1 Fourier Analysis Of The Radiative Transfer Equation 92
A.2 Fourier Analysis Of The Radiative Transfer Equation With Diffusion Equation 94
A.3 Solution Of Radiative Transfer Equation 98
A.4 Derivation Of Discretized Form Of The Diffusion Equation 100
A.5 Derivation Of Discretized Form Of The Grey Equation 103
A.6 Boundary Conditions Of The Diffusion Equation 108
A.7 Boundary Conditions Of The Grey Equation 111
A.8 Solution Of The Diffusion And The Grey Equations 112

B. MARCHAND'S MODEL 115

C. LEE'S RADIATIVE TABLES 120

D. LISTING OF THE RADIATION TRANSPORT CODE 122

ACKNOWLEDGEMENT

I would like to express my sincere gratitude to Dr. C.E. Capjack and Dr. C.R. James for their financial support. I also like to thank Dr. C.E. Capjack and Dr. R. Rankin for bringing to my attention the Diffusion Synthetic Acceleration method and for their encouragement and supervision of this project.

Mr. D. Vick provided much helpful advice and suggestions and was always available for discussion. I would like to express my thanks to him. Dr. Marvin, from Lawerence Livermore National Laboratory, USA, was very helpful in deriving boundary conditions for the diffusion equation. In his absence, I like to express my appreciation for the discussion and correspondence that he provided.

I also like to thank my brother Hamid Butt for the computer (which was used for developing the code for the model problem) and the technical support for maintaining it.

ABSTRACT

The main objective of this research is to incorporate the effects of radiation transport into MEDUSA, a code used at the University of Alberta and other research laboratories to study laser plasma interaction phenomena. The effects of radiation transport on ablation pressure and the ablation mass are investigated. When radiation transport is included, the amount of laser energy that is available for ion, kinetic and thermal energies changes. This change in energy is also investigated. The solution of the radiative transfer equation for a one dimensional slab geometry is obtained by using a neutronic transport technique known as **DIFFUSION SYNTHETIC ACCELERATION (DSA)**. The secondary objective of this research is to corroborate the validity of the simplified algorithm developed by Marchand et al at the University of Alberta. The radiation transport algorithm is developed taking into consideration its eventual extension to two dimensional geometries. However, the extension to higher dimensions is not the objective of the present research.

CHAPTER ONE
INTRODUCTION

1.1 LASER DRIVEN NUCLEAR FUSION:

In early 1970, many researchers argued that one could use lasers as a mean of igniting thermonuclear fusion[1/1]. They showed theoretically that a thin shell filled with a deuterium-tritium mixture can be compressed to many times its solid density through laser driven ablative implosion. In an ablative implosion only the exterior of the shell is heated. The shell is shocked, compressed and driven toward the origin by the reaction force produced by the material streaming off. In this way fuel inside the shell can be brought to the densities required for thermonuclear fusion.

During compression, the heated fuel pellet emits electromagnetic radiation which can significantly influence the compression efficiency. These emitted photons can preheat the uncompressed target core, thereby reducing the final target compression. This in turn degrades the pellet gain. Therefore, it is of considerable importance to know the temperature on the inside of the target shell. Such knowledge allows one to choose the proper isentrope for compression calculations as well as to check the predictions of detailed numerical simulations of laser driven implosions. If preheating is sufficiently strong, it is possible that fuel may not ignite. Therefore, it is essential to minimize the fuel preheating during the implosion phase.

When the laser intensity is in the range of 10^{16} to 10^{18} W m^{-2}, energy transport due to radiation can exceed heat conduction due to other processes. Experiments[1/2] have shown that up to 25% of the laser input energy can be lost through radiative emission. From these experiments it can be concluded that by neglecting radiation transport, one may be omitting a significant energy loss mechanism. Therefore, a computer simulation without radiation transport may not yield results that are consistent with experimental observations. Radiation transport is a very complex

process due to its nonlinear nature and because of the dependence of the radiation field on space, angle, frequency and time. A treatment of the interaction of the radiation field with atoms requires a detailed knowledge of various coefficients such as the atomic population densities, the absorption coefficient and emissitivity. Despite its complexity, it is essential to include at least a qualitative analysis of radiation transport in any computer simulation.

1.2 PHYSICS OF LASER PRODUCED PLASMA:

A detailed analysis of all of the processes taking place in a laser produced plasma is beyond the scope of this thesis. In this section, a brief summary of some of the processes which take place when a laser beam is incident on matter are discussed.

When a laser impinges on a target surface, it is initially absorbed by the production of photoelectrons. This leads to electron ionization and heating of the target. The target material evaporates, the vapour is ionized by collisions and a plasma layer is formed. If the intensity of the laser beam is sufficiently high the electronic field of the incident laser beam can lead to noncollisional heating and an outward acceleration of the plasma in an explosive manner. The plasma layer expands mostly in an outward direction while heat is conducted into the solid. This inward heat conduction leads to further evaporation of the target layer. This is called **ablation** of the target material. The momentum of the ablated plasma is balanced by momentum of the solid target. The momentum transferred by the action of the ablation pressure and the effect of the pondermotive force, launches a shock wave in the solid which after a short time overtakes the front of the heat wave. Assuming classical theory of heat conduction, this time is given as[1/3]

$$t_o = b\left(\frac{M}{2k}\right)^{\frac{3}{2}}\left(\frac{3}{2}kN\right)^{-2}\phi$$

where ϕ is the flux, N is the ion density, M is the atomic mass of the target, k is the Boltzmann constant and b is $2.0E^{-13}$ If the laser pulse is short compared to t_o the

heated matter has no time to move and energy diffuses into the target by heat conduction. On the other hand, if the laser pulse lasts for a time longer than t_o then expansion is important while laser energy is being absorbed. When the laser pulse is very long compared to t_o the plasma can be divided into three phases. Phase 0 has a mass density ρ_o of the undisturbed solid. Phase 1 has mass density ρ_1 and is called the dense phase of opaque ionized matter which is heated by the shock wave. This mass penetrates into phase 0 with the speed of the shock. Phase 2 is composed of plasma subliminated from the boundary of phase 1.

Two thermodynamic quantities, pressure and energy, directly govern the hydrodynamics of the plasma. The energy deposited by the laser pulse can be used to determine the temperature of the plasma and from this one can deduce the pressure. The pressure drives the expansion of the plasma and determines the strength of the recoiled shock launched into the solid and thereby establishes the implosion velocity of the plasma.

A plasma can be considered as either nonideal or ideal. In a nonideal plasma ($Q<Z$ where Q is the ion charge and Z is the atomic number) matter is partially ionized. The coulomb interaction is strong in this case and free electrons can exist in degenerate form. The ideal plasma ($Q=Z$) is fully ionized and the electrical interaction is weak due to the screening clouds around charges. The screening energy increases as the temperature is reduced and eventually exceeds kT. When this happens a strongly coupled plasma is formed which is nonideal. An approximation for the ionization energy is given as

$$I = 13.6 \left(\frac{Q}{n}\right)^2 \quad ev$$

where n is the principle quantum number of the outer most electron. The above expression shows that higher Z plasmas are more difficult to ionize. An ideal plasma emits radiation by bremsstrahlung, radiative recombination and line radiation from hydrogen like or helium like ions. In a magnetically confined plasma with high Z, the bremsstrahlung radiation can become an important mechanism for cooling. For

low density plasma, radiation freely escapes and it can be used to infer parameters such as the plasma density and temperature. In a partially ionized plasma, radiation is strongly absorbed by the bound electrons and the photon population builds up toward a black body distribution.

When a laser beam is incident on a material, the energy that is absorbed by free electrons leads to an increase in their temperature. An increase in temperature increases the Debye length which increases the ion interaction. This forces ions to redistribute so as to reach equilibrium. As plasma is heated, different types of emission spectra are observed. The continuum emission spectrum reflects the energy spectrum of the free electrons. The energetic x-ray signals indicate the presence of super-thermal electrons.

In a plasma, hot regions radiate strongly and emitted photons transport energy to cooler parts of the plasma or permit energy to escape altogether. Since radiation travels rapidly, it plays an important role in plasma hydrodynamics. The radiation that is emitted and absorbed is due to many different processes which take place at a subatomic level. Some of the important processes are discussed below.

Bremsstrahlung Emission: In bremsstrahlung emission, radiation is emitted when electrons are scattered by atoms and ions. As electrons approach a nuclei they are deaccelerated and radiation is emitted.

Free-Free absorption: Absorption of a photon by a free electron is known as free-free absorption. The electron absorption cross-sectional area is obtained by using the principle of balance which states that at thermal equilibrium, the absorption rate is equal to the rate of emission and is given as[1/3]

$$\sigma^{B} = \frac{8\pi^3}{3\sqrt{3}} Z^2 a_o^5 \left(\frac{e^2}{a_o h\nu}\right)^3 \frac{e^2}{a_o \epsilon}$$

where Z is the atomic number, e is the electron charge, h is the Planckian constant, a_o is the radiation constant (=7.5607E-16), ϵ is the permeability constant of the plasma and ν is the frequency.

Radiative Recombination: Radiative recombination occurs when

free electrons radiate more energy than their initial kinetic energy. At negative energies these electrons are trapped in bound states.

Photoelectric Effect: Here, a bound electron absorbs a photon and moves to a higher state.

Line Emission: Line emission occurs when a bound electron in an upper state spontaneously emits a photon of energy hν and falls into a lower state.

In a laser heated plasma, energy is deposited primarily into the electrons and the rate at which the electrons in turn transport this energy to higher density colder plasma determines both the efficiency of implosion and the plasma conditions in the region of deposition.

Mechanisms which are generally associated with the heating of the pellet are:

1. Classical electron thermal conduction.
2. Radiation transport.
3. Super thermal electron transport.
4. Shock waves.

Classical conduction is always present, and is modified by anomalous effects from ion and magnetic field fluctuations[1/4]. When excessive energy is deposited to thermal electrons during an implosion, the classical conduction wave burns through the shell, leading to preheating of the pellet. This condition can be readily avoided with proper pulse shaping. Radiative preheating arises from the reabsorption of bremsstrahlung, recombination and line radiation photons near the ablation surface where plasma electrons are typically in the range of 300 to 500 ev[1/5]. Super thermal electrons are generated when various thresholds for the absorptive instabilities are exceeded[1/6]; for example, resonant absorption readily furnishes 100 keV electrons with 10.6 μm laser light intensities of 10^{20} W m^{-2}. Shock waves[1/7] leads to large temperature gradients. They play an important role when thicker targets are used. At intermediate irradiance (10^{16} to 10^{17} W m^{-2}) the dominant heat transport mechanism can be radiation transport.

The effects of radiation transport have been experimentally investigated by

many researchers[1/8,9]. In numerous experiments, different pellet materials have been used in order to observe the effects of radiation transport in low and high Z materials. Duston et al[1/2,8] used carbon as a target material, and rejected the common notion that for lower Z material radiation transport is negligible. This notion was due to the assumption that for lower Z materials the bound electrons would be easily stripped off and therefore radiation would make a negligible contribution to plasma dynamics and energy transport in these targets. Yaakobi et al[1/9] have shown that use of a low Z (plastic) coating reduces the preheating, thus leading to a higher density ablative implosion.

1.3 OBJECTIVE AND ORGANIZATION OF THE THESIS:

When a laser beam is incident on a target, radiation is emitted and then transported and reabsorbed in the target. This can significantly affect the hydrodynamics of the target and ablation parameters. In laser fusion, a precise knowledge of these parameters is crucial for target design. Even though our research does not involve laser induced nuclear fusion, inclusion of radiation transport is useful for a better understanding of radiative effects in other problems, such as use of emitted radiation as a source of x-rays[1/10] for lithography applications. Therefore, by including radiation transport in MEDUSA, the behavior of laser heated plasma can be better understood. The Diffusion Synthetic Acceleration technique is used to implement the radiative transfer equation in the MEDUSA code. The main objectives of the present research are:

i. To develop an algorithm which can be extended to solve the radiative transfer equation in two dimensions.

ii. To corroborate Marchand's algorithm.

The thesis consists of five chapters. In Chapter One, the importance of the understanding of radiation relevant to laser driven nuclear fusion is discussed, followed by a prologue to the processes involved in laser plasma interactions. In Chapter Two, the derivation and validity of the radiative transfer equation are

discussed. Chapter Three includes a detailed analysis of the Diffusion Synthetic Acceleration Scheme (**DSA**). Chapter Four includes simulations with the radiation code when a model problem is used to test the validity of the DSA model. Chapter Five contains MEDUSA simulations using Marchand's model and the present model. The main objective is to present a comparison between Marchand's model and the Diffusion Synthetic Acceleration model.

Finally, a detailed analysis of the equations involved in the Diffusion Synthetic Acceleration model is included in Appendix A. This includes a Fourier stability analysis (where possible), the discretization of all equations involved in the algorithm, and a discussion of the boundary conditions. Marchand's model, currently used in MEDUSA to study radiative effects in laser produced plasma is reviewed in Appendix B. In Appendix C, a brief discussion is presented of the atomic physics data used in MEDUSA. A copy of the radiation transport code is included at the end of the thesis in Appendix D.

CHAPTER TWO
RADIATIVE TRANSFER EQUATION

2.1 DERIVATION OF RADIATIVE TRANSFER EQUATION:

The radiative transfer equation represents the various processes that take place in a plasma at a sub-atomic level. These processes lead to the generation and transport of radiation, resulting in a change in the number of photons in a given region. The time rate of change of the photons in a volume ΔV is given by

$$\frac{\partial[f(r,\nu,\Omega,t)\Delta V]}{\partial t} = \Delta V \frac{\partial[f(r,\nu,\Omega,t)]}{\partial t} \qquad (2.1.01)$$

where $\Delta V = \Delta x \Delta y \Delta z \Delta\mu \Delta\varphi$ and f is the distribution function. Physically f is defined such that the number of photons at a given time t at a location in space **r** in a differential volume element **dr** with frequency interval dν travelling in direction Ω in a solid angle interval dΩ is

$$dn = f\, dr\, d\nu\, d\Omega$$

This time rate of change of photons in a volume element ΔV depends on:

1. Net rate of streaming of photons out of a volume through the bounding surface.
2. Absorption of photons within the volume element.
3. Emission of photons from the volume element.
4,5. Scattering into and out of the volume element.

A detailed description of the physical interpretation of the above processes can be found elsewhere[2/1]. In this section, they are discussed briefly in order to derive the radiative transfer equation.

1. The rate of photon loss through the surface of a cube perpendicular to the x-axis is

$$streaming_x = \dot{x}f(r,\nu,\Omega,t)]_x^{x+\Delta x}\Delta y\Delta z\Delta\nu\Delta\mu\Delta\varphi = \Delta V\frac{\partial}{\partial x}[\dot{x}f(r,\nu,\Omega,t)] \tag{2.1.02}$$

where x denotes the x-components of the photon velocity and $\Delta y\Delta z\Delta\mu\Delta\varphi$ is the appropriate surface area. From this one can determine the net rate of streaming from the cube to be

$$streaming = \Delta V\left[\frac{\partial(\dot{x}f)}{\partial x}+\frac{\partial(\dot{y}f)}{\partial y}+\frac{\partial(\dot{z}f)}{\partial z}+\frac{\partial(\dot{\nu}f)}{\partial\nu}+\frac{\partial(\dot{\mu}f)}{\partial\mu}+\frac{\partial(\dot{\phi}f)}{\partial\varphi}\right] \tag{2.1.03}$$

where μ and φ derivatives represent the rate of change of photons in the directions μ and φ (the polar angle with respect to z-axis and the azimuthal angle with respect to the horizontal axis), respectively.

2. The rate of absorption is equal to the product of the number of photons in the volume element ΔV and the probability of absorption per photon per unit time

$$\text{rate of absorption} = c\sigma_a f\Delta V \tag{2.1.04}$$

where σ_a is the absorption coefficient.

3. The photon emission rate is equal to the spontaneous rate of emission divided by the energy of the photon

$$\text{photon emission rate} = S\Delta V/h\nu \tag{2.1.05}$$

where S is the rate of energy emission due to spontaneous processes.

4. The rate of out-scattering from the volume element is

$$c\Delta V\int_0^\infty d\hat{\nu}\int_{4\pi}d\hat{\Omega}\sigma_s(r,\nu\rightarrow\hat{\nu},\Omega.\hat{\Omega},t)\,f\,(r,\nu,\Omega,t)$$

5. The rate of in-scattering to the volume element is

$$c\Delta V\int_0^{\infty}d\acute{\nu}\int_{4\pi}d\acute{\Omega}\,\sigma_s(r,\acute{\nu}\rightarrow\nu,\acute{\Omega}.\Omega,t)\,f\,(r,\acute{\nu},\acute{\Omega},t)$$

(2.1.06;07)

In the above equations, σ_s is the scattering coefficient and c is the speed of light.

The equation of radiative transfer is obtained by summing the above equations with appropriate signs to designate a loss or gain. The resultant equation is

$$\frac{\partial f(\nu,\Omega)}{\partial t}+\frac{\partial(\dot{x}f)}{\partial x}+\frac{\partial(\dot{y}f)}{\partial y}+\frac{\partial(\dot{z}f)}{\partial z}+\frac{\partial(\dot{\nu}f)}{\partial \nu}+\frac{\partial(\dot{\mu}f)}{\partial t}+\frac{\partial(\dot{\phi}f)}{\partial \varphi}$$
$$=\frac{S(\nu)}{h\nu}-c\sigma_a(\nu)f(\nu,\Omega)+c\int_0^{\infty}d\acute{\nu}\int_{4\pi}d\acute{\Omega}\,\sigma_s(\acute{\nu}\rightarrow\nu,\acute{\Omega}\bullet\Omega)f(\acute{\nu},\acute{\Omega})$$
$$-c\int_0^{\infty}d\acute{\nu}\int_{4\pi}d\acute{\Omega}\,\sigma_s(\nu\rightarrow\acute{\nu},\Omega\bullet\acute{\Omega})f(\nu,\Omega)$$

(2.1.08)

Equation (2.1.08) can be simplified by assuming that photons stream in straight lines. When this assumption is made, $\partial x/\partial t = c\Omega_x$, since photons travel with speed c in a given direction. Similar expressions can be obtained for the y,z axes. Since there is no change in frequency as photons stream, $\partial\nu/\partial t = 0$. Further, $\partial\mu/\partial t=\partial\varphi/\partial t=0.0$, since these angles are measured with respect to fixed axes in space. The distribution function f is related to the specific intensity as $I=ch\nu f$. Then with the above assumptions, equation (2.1.08) in terms of the specific intensity reduces to

$$\frac{1}{c}\frac{\partial I(\nu,\Omega)}{\partial t}+\Omega\bullet\nabla I(\nu,\Omega) = S(\nu)-\sigma_a(\nu)I(\nu,\Omega)$$
$$+\int_0^{\infty}d\acute{\nu}\int_{4\pi}d\acute{\Omega}\left[\frac{\nu}{\acute{\nu}}\sigma_s(\acute{\nu}\rightarrow\nu,\acute{\Omega}\bullet\Omega)I(\acute{\nu},\acute{\Omega})-\sigma_s(\nu\rightarrow\acute{\nu},\Omega\bullet\acute{\Omega})I(\nu,\Omega)\right]$$

(2.1.09)

It can be shown[2/1] that when induced processes are included, the processes of emission and scattering are enhanced by the factor

$$\left[1+\frac{c^2I}{2h\nu^3}\right]$$

This enhancement leads to nonlinearity (in the form of I^2) in the transfer equation

in the following form

$$\frac{1}{c}\frac{\partial I}{\partial t} + \Omega.\nabla I = \acute{\sigma}_e\,[B-I] + \int_0^{\infty} d\acute{\nu}\,\frac{\nu}{\acute{\nu}}\int_{4\pi} d\hat{\Omega}\,\sigma_s \acute{I}\,[1+\frac{c^2 I}{2h\nu^3}] - \int_0^{\infty} d\acute{\nu}\int_{4\pi} d\hat{\Omega}\,\sigma_s I\,[1+\frac{c^2 \acute{I}}{2h\acute{\nu}^3}]$$

$$\text{where} \qquad S=\acute{\sigma}_e B \qquad \text{and} \qquad \acute{\sigma}_e=\sigma_e[1+\frac{c^2 B}{2h\nu^3}] \tag{2.1.10}$$

Here, for simplicity the notations of I and σ_s are given as

$$I = I\,[r,\nu,\Omega,s] \qquad \text{and} \qquad \acute{I} = I\,[r,\acute{\nu},\hat{\Omega},s]$$

This nonlinearity severely limits one's ability to solve the transfer equation. Therefore, equation (2.1.10) is further simplified by assuming that there is no change in frequency upon scattering. With this assumption the induced in- and out-scattering contribution completely cancel each other, and the resulting equation is simply

$$\frac{1}{c}\frac{\partial I}{\partial t} + \Omega.\nabla I = \acute{\sigma}_e[B - I] \tag{2.1.11}$$

This equation forms the basis of the present research. The goal is to find a technique which can efficiently solve this equation. It is important to briefly discuss the validity of the radiative transfer equation, before we discuss the method used to solve the radiative transfer equation.

2.2 THE VALIDITY OF THE RADIATIVE TRANSFER EQUATION:

Many aspects of radiation transport were ignored when the radiative transfer equation was derived above. Some of them are beyond the scope of the present research and some are irrelevant to the objectives of the present research. In this section, approximations that are used in the derivation of the above transfer equation

are briefly discussed.

There are two classes of approximation: those which are inherent in any radiative transfer equation and those which can be incorporated at the expense of simplicity.

The radiative transfer equation was derived using the assumption that photons are particles. However, it is well known that photons exhibit wave behavior, that is in reality a photon is a wave packet. By treating photons as particles, one intrinsically is neglecting the effects of interference, diffraction and reflection in radiation transport. In the radiative transfer equation, one deals with intensities rather than amplitudes, hence interference is nonexistent. This requires that the density of photons be sufficiently low so that overlap of the tails of the wave packets is negligibly small. Photons of sufficiently different frequencies do not interfere even when they coincide spatially; in other words, photons in the transfer equation are incoherent. It is further assumed that collision and emission processes occur instantaneously. That is, the loss or gain of photons due to these processes is characterized by σ_a, σ_s and B (absorption and scattering coefficient and the emissivity respectively) at a given instant of time rather than being dependent upon some sort of time average of these quantities over the collision or emission time. Finally, the diffraction and reflection wave behaviour of photons can not be manifested in any radiative transfer equation; since it requires that scattering centres be correlated as in a crystal and the spatial extent of wave packet be such that several scattering centres are encompassed by a photon. Therefore, in the transfer equation we treat scattering as independent and isolated events; in other words we assume scattering centres are randomly distributed or the wave packets are small compared to the distance between the scattering centres. This further implies that photons have no preferred direction.

The approximations discussed so far are inherent to all transfer equations of photons. The approximations which remain to be discussed are assumed in deriving the radiative transfer equation (2.1.08) and can be incorporated into the equation (2.1.08) at the expense of simplicity.

The two states of polarization of a photon can be added into the radiative transfer equation; this results in four transfer equations which in general are coupled. In practice photons do not move in straight lines since the refractive index is a function of position. If the refractive index is a function of time as well, then a photon changes its frequency as it streams between collisions. One can incorporate[2/1] refractive and dispersion effects into the streaming term of the transfer equation. Finally, σ_s and S are assumed to be angularly independent in (2.1.08), this implies no inherent preferred direction in the matter. However, in radiative hydrodynamic problems the material in question is normally moving. Therefore, as seen by an inertial frame observer, this motion does introduce a preferred direction, namely the direction of motion of the fluid. These angular dependence properties are not inherent properties of the material, but arise due to relative motion between the fluid and the observer. These are computed using the special theory of relativity. These angular effects are of the order of (u/c), where u is the speed of the fluid and c the speed of light; therefore, one can normally neglect the angular dependence in quantities such as the radiation intensity for nonrelativistic velocities.

CHAPTER THREE
DIFFUSION SYNTHETIC ACCELERATION

3.1 INTRODUCTION:

There are many classical methods, such as the Eddington Approximation, Asymptotic Diffusion Theory, the P-N Approximation[3/1] and the Monte Carlo Method[3/2] which have been used in the past to solve the radiative transfer equation. These methods are either too crude or are computationally inefficient. Since the late 1960's, researchers have been investigating other options for solving the radiative transfer equation. One of the most popular techniques is Synthetic Acceleration. This is sometimes used to solve neutronic transport problems, but due to its slow convergence for radiative transport problems it was not attractive. In the late 1970's and early 1980's this technique was greatly improved (by acceleration of the diffusion equation with the grey equation) and today is one of the most efficient methods of solving radiation transport problems in one dimension. The successful implementation of this method for a model problem at Lawrence Livermore National Laboratory was the main motivation for the development of the present code. Diffusion Synthetic Acceleration (**DSA**) is the main topic of this thesis, since it can have ambiguities in its formulation, a great deal of effort has been made to ensure that important aspects of the DSA technique relevant to one dimensional slab geometry are well explained.

3.2 BRIEF HISTORY:

In 1963, Kopp[3/3] reported that one can improve the spectral radius of the **source iteration** technique (also known as **power** or **lambda iteration**) by using a synthetic acceleration method. In synthetic acceleration one solves a low order form of the original equation to update the source term of the original equation for the

next iteration. For example, the diffusion equation can be treated as a low order form of the transfer equation; the difficult part is to find the form of the low order equation which reduces the spectral radius and remains stable. The significant improvement and stability issues were not resolved until the late 1970's. In 1977, Alcouffe[3/4] reported the cause of instability and proved that the solution for DSA was unstable for cells with large width because the discretized form of the low order equation was not derived from the discretized form of the original equation. In 1985, Alcouffe et al[3/5] successfully reported on the implementation of the DSA method for a radiative model problem. The code presented here is similar to the work they published in 1985 with minor modifications. The DSA technique like any other method for radiative problems comes with its limitations. When it works, it is very efficient compared to the source iteration or to other known methods for one dimensional problems. Its efficiency degrades for higher dimensional and curvilinear geometry problems. These instability concerns have been eliminated to a great extent with the use of finite element discretization instead of finite difference discretization of the transfer equation in space.

3.3 DISCRETIZATION OF THE TRANSFER EQUATION:

The radiative transfer equation and the energy balance equation are solved simultaneously (this formulation allows us to test our code against a Marshak Wave Bench Mark). The equations for a one dimensional slab geometry are given by[3/5]

$$\frac{1}{c}\frac{\partial I}{\partial t}(x,\nu,\mu,t) + \mu\frac{\partial I}{\partial x}(x,\nu,\mu,t) + \sigma(x,\nu)I(x,\nu,\mu,t) = S(\nu,T) = \sigma(\nu,T)B(\nu,T)$$

$$\frac{\partial u_r(T)}{\partial t} = \beta(T)\left[\int_0^\infty \sigma(\nu,T)I_0(x,\nu,t)d\nu - c\sigma_p(T)u_r(T) + S_{ext}\right]$$

$$\text{where} \quad u_r = \frac{c}{4\pi}\int_0^\infty B\,d\nu \quad \sigma_p = \frac{\int_0^\infty \sigma B\,d\nu}{\int_0^\infty B\,d\nu} \quad \beta = \frac{4aT^3}{c_v}$$

(3.3.01;02;03a,b,c)

Where I is the specific intensity of radiation, defined as the amount of radiative

energy transferred across a surface element ds with normal **n** at point x, in frequency range of dν about ν, in an angle dμ about μ in time interval dt about t. The energy emission rate due to spontaneous processes is given by S; B is the emissivity, T is the material temperature, σ is the absorption coefficient defined such that the probability of a photon being absorbed in a distance ds is σds, c_v is the material specific heat per unit volume, a is the radiation constant, S_{ext} is the external source in the slab, u_e is the radiative energy density and I_o is the scalar intensity and is defined as

$$I_o(x,\nu,t) = \int_{-1}^{1} I(x,\mu,\nu,t)\, d\mu \qquad (3.3.04)$$

3.3.1 DISCRETIZATION IN TIME:

The radiative transfer equation and the energy balance equation are discretized in time using a backward Euler time differencing scheme in order to ensure stability. The dependence of variables on frequency, angle, space and time is omitted for simplicity. The discretized form of (3.3.01,02,03) in time is given as

$$\frac{1}{c\Delta t^n}(I^{n+1}-I^n) + \mu\frac{\partial I^{n+1}}{\partial x} + \sigma^* I^{n+1} = \sigma^* B^{n+1}$$

$$\frac{1}{\Delta t^n}(u_e^{n+1}-u_e^n) = \beta^*\left[\int_0^\infty \sigma^* I_0^{n+1} d\nu - c\sigma_p^* u_e^{n+1} + S_{ext}\right]$$

$$u_e^{n+1} = \frac{c}{4\pi}\int_0^\infty B^{n+1}\, d\nu \qquad (3.3.05;06;07)$$

The quantities with * superscript are computed using the temperature at time step n, since the temperature at time step (n+1) is not known. In addition, the following approximation to the function B is used[3/6]

$$B^{n+1} = \frac{c}{2}u_e^{n+1} b(\nu,T^*) \qquad \textit{subject to} \qquad \int_0^\infty b(\nu,T)\, d\nu = 1 \qquad (3.3.08)$$

By using (3.3.07) and (3.3.08) and assuming that the external source is zero, the function B reduces to

$$B^{n+1} \approx \frac{cb^*}{2}\frac{[\beta^*\Delta t^*\int_0^\infty \sigma^* I_o^{n+1} d\nu + u_e^n]}{(1+c\Delta t^n\beta^*\sigma_p^*)}$$

$$= \frac{\chi\eta}{2}\left[\int_0^\infty \sigma^* I_0^{n+1} + \frac{u_e^n}{\beta^*\Delta t^n}\right]$$

$$\text{where} \quad \alpha = \frac{1}{\beta^*\sigma_p^*}, \quad \tau^n = \frac{1}{c\Delta t^n}, \quad \chi = \frac{\sigma^* b^*}{\sigma_p^*}, \quad \eta = \frac{1}{(1+\alpha\tau)}$$

(3.3.09;10a,b,c,d)

With these relations, equations (3.3.06;07) reduce to

$$\mu\frac{\partial I^{n+1}}{\partial x} + (\sigma^*+\tau)I^{n+1} = \frac{\chi\eta}{2}\left[\int_0^\infty \sigma^* I_0^{n+1} d\nu + \frac{u_e^n}{\beta^*\Delta t^n}\right] + \tau^n I^n$$

$$u_e^{n+1} = \frac{\eta}{2}\left[\int_0^\infty \sigma^* I_o \, d\nu + \frac{u_e^n}{\Delta\beta^*}\right]$$

(3.3.11a,b)

If the time index is suppressed in the radiative transfer equation(3.3.11a), it reduces to

$$\mu\frac{\partial I}{\partial x} + (\sigma+\tau)I = \frac{\chi\eta}{2}\int_0^\infty \sigma I_0 d\nu + Q$$

(3.3.12)

where Q contains all the terms evaluated at the previous time step and remains unchanged while the transfer equation is being solved iteratively. Q is given as

$$Q = \frac{\chi^*\eta}{2}\frac{u_e^n}{\beta^*\Delta t^n} + \tau^n I^n$$

(3.3.13)

3.3.2 DISCRETIZATION IN FREQUENCY:

We use equation (3.3.12) to discretize the radiative transfer equation in

frequency. The discretized form of the equation is obtained by integrating (3.3.12) over the frequency interval dν as shown below

$$\int_{\nu_l}^{\nu_h} \mu \frac{\partial I}{\partial x}\, d\nu + \int_{\nu_l}^{\nu_h} (\sigma+\tau) I \, d\nu = \int_{\nu_l}^{\nu_h} \frac{\chi\eta}{2} \int_0^{\infty} \sigma I_0 \, d\nu + \int_{\nu_l}^{\nu_h} Q \, d\nu$$

(3.3.14)

If we define

$$I_g = \int_{\nu_l}^{\nu_h} I \, d\nu \qquad Q_g = \int_{\nu_l}^{\nu_h} Q \, d\nu \qquad \sigma_g = \frac{\int_{\nu_l}^{\nu_h} \sigma I \, d\nu}{\int_{\nu_l}^{\nu_h} I \, d\nu} \qquad \chi_g = \int_{\nu_l}^{\nu_h} \chi \, d\nu$$

(3.3.15a,b,c,d)

then the multi-group transfer equation can be expressed as

$$\mu \frac{\partial I_g}{\partial x} + (\sigma_g+\tau) I_g = \frac{\chi_g \eta}{2} \Sigma_g \, \sigma_g I_{0g} + Q_g$$

(3.3.16)

3.3.3 DISCRETIZATION IN ANGULAR SPACE:

The discretized form of the radiative transfer equation (3.3.16) in angular space is obtained by integrating in angular space as defined below

$$\mu_m \frac{\partial I_{mg}}{\partial x} + (\sigma_g+\tau) I_{mg} = \frac{\chi_g \eta}{2} \Sigma_g^G \, \sigma_g I_{0g} + Q_{mg}$$

$$\textit{where} \qquad I_{0g} = \Sigma_{m=1}^{M} I_{mg} \omega_m$$

$$I_{mg} = \frac{1}{\Delta \omega_m} \int_{\omega_{m-\frac{1}{2}}}^{\omega_{m-\frac{1}{2}}} I_g \, d\omega_m$$

$$\textit{subject to} \qquad \Sigma_{m=1}^{M} \omega_m = 2$$

(3.3.17a,b,c)

Physically I_{mg} represents the specific intensity in a particular direction with weight distribution of ω_m , μ_m is the cosine angle of the specific intensity with respect to the

x-axis and M is the total number of discretized angles.

3.3.4 DISCRETIZATION IN SPACE:

The spatial discretization of the radiative transfer equation (3.3.17a) is obtained by integrating in space over the cell width, as shown below

$$I_{mgi} = \frac{1}{\Delta x_i}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} I_{mg}dx$$

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\mu_m\frac{\partial I_{mg}}{\partial x}dx + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}(\sigma_g+\tau)I_{mg}dx = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\frac{\chi_g\eta}{2}\Sigma_g\sigma_g J_{0g}dx + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}Q_{mg}dx$$

(3.3.18)

then the transfer equation reduces to

$$\frac{\mu_m}{\Delta x_i}(I_{mgi+\frac{1}{2}} - I_{mgi-\frac{1}{2}}) + (\sigma_{gi}+\tau)I_{mgi} = \frac{\chi_{gi}\eta_i}{2}\ \Sigma_g\ \sigma_{gi}J_{0gi} + Q_{mgi}$$

(3.3.19)

3.4 SOURCE ITERATION:

Equation (3.3.19) is simply a set of (M*G) transfer equations corresponding to M angles and G frequency groups. This equation includes three unknowns I_{mgi} and $I_{mgi\pm1/2}$, where one of $I_{mgi\pm1/2}$ is obtained from the boundary condition of the cell. Very often one uses a relation known as Diamond Differencing (**DD**) to equate the number of equations with the number of unknowns. This relation is given as,

$$I_{mgi} = \frac{1}{2}(I_{mgi+\frac{1}{2}} + I_{mgi-\frac{1}{2}})$$

(3.4.01)

This simply states that the intensity at the centre of a cell is equal to the average of the intensity at the cell boundaries. The difficulty in solving the radiative transfer equation arises due to the coupling (summation over the frequency groups) of the specific intensity on the right hand side of (3.3.19). The simplest approach to solve

such types of equations is by the use of the source iteration technique. This involves making an initial guess for the source term in equation (3.3.19) and solving for the intensities. The solution is then taken to be the new initial guess in the source term (the summation term on right hand side) of (3.3.19) for the next iteration and equation (3.3.19) is solved again. This is repeated until the new solution and initial guess have converged to some desired accuracy. The final form of the set of equations involved in the source iteration (SI) method is written as

$$\mu_m(I^{l+\frac{1}{2}}_{mgi+\frac{1}{2}} - I^{l+\frac{1}{2}}_{mgi-\frac{1}{2}}) + \hat{\sigma}_{gi} I^{l+\frac{1}{2}}_{mgi} = \frac{\eta \chi_{gi} \Delta x_i}{2} \Sigma_g \sigma_{gi} I^l_{0gi} + \Delta x_i Q_{mgi}$$

$$\text{where} \qquad \hat{\sigma}_{gi} = (\sigma_{gi} + \tau)\Delta x_i$$

$$I^{l+\frac{1}{2}}_{mgi} = \frac{1}{2}[I^{l+\frac{1}{2}}_{mgi+\frac{1}{2}} + I^{l+\frac{1}{2}}_{mgi-\frac{1}{2}}]$$

$$I^{l+\frac{1}{2}}_{0gi} = \Sigma_m I^{l+\frac{1}{2}}_{mgi} \omega_m$$

(3.4.02a,b,c)

In the SI method one uses (3.4.02) to obtain the intensity as is shown in the appendix (section A.3). A Fourier stability analysis of the transfer equation shows that when $\tau \to 0$ or/and $\sigma \gg 1$, the spectral radius can be arbitrarily close to unity. In simple terminology, it means that the error reduction per iteration can be extremely slow or that an infinite number of iterations may be required. However, in practice when the radiative transfer equation is fully discretized and one has a finite frequency range rather than from 0 to ∞, the radius of convergence can shown to be always less than one. This is due to the fact that for a finite system all of the Fourier modes are not present. This slow convergence compels one to look for other methods which can reduce the spectral radius. The next section deals with this issue.

3.5 DIFFUSION SYNTHETIC ACCELERATION OF THE TRANSFER EQUATION:

3.5.1 INTRODUCTION TO SYNTHETIC ACCELERATION:

The idea behind synthetic acceleration can be explained as follows[3/7]. Suppose

we are given an equation of the form

$$[A\text{-}B]f = S$$

where [A-B] is difficult to invert, but A can be inverted relatively easily. We try the following iteration strategy

$$f^{l+1} = A^{-1} Bf^{l} + A^{-1} S$$

where l and l+1 are iterative indices and the eigen value of $[A^{-1}B]$ determines the rate of convergence. The above iteration scheme will converge as long as the spectral radius (the largest eigenvalue) is less than one. It can be shown that one can solve above problem iteratively as

$$[A\text{-}B](f - f^{l+1}) = B\,(f^{l+1} - f^{l})$$

where f is the converged solution. The above equation implies that an exact solution can be obtained immediately by inverting [A-B] if the solution to f^{l+1} is known. The inversion of [A-B] is the obstacle we are trying to remove, so we are no closer to the resolution of the problem. If we assume that L is an approximation to [A-B] and if L is easily invertible, then the problem can be solved in two steps as given below

$$f^{l+1/2} = A^{-1} Bf^{l} + A^{-1} S$$

$$L(f^{l+1} - f^{l+1/2}) = B(f^{l+1/2} - f^{l})$$

This iteration strategy is called synthetic acceleration. In order to elucidate the use of synthetic acceleration, let us consider the radiative transfer equation. The radiative transfer equation and its low order form corresponding to the above set of equations is given by

$$(\mu\frac{\partial}{\partial x}+\sigma)I^{l+\frac{1}{2}}=\frac{\chi\eta}{2}\Sigma_g\Sigma_m\sigma I^{l}+Q$$

$$L(I^{l+1}-I^{l+\frac{1}{2}})=\frac{\eta\chi}{2}\Sigma_g\Sigma_m\omega_m\sigma_g(I^{l+\frac{1}{2}}-I^{l})$$

It is trivial to identify A and B, but L is not so obvious. The main task in synthetic acceleration is to find the operator L, which reduces the spectral radius and yields a stable solution. We will show by using a systematic approach that the required operator is the diffusion operator. In early 1980, Larsen[3/8] developed a four step procedure whereby one could derive beginning with virtually any differencing

scheme of the transfer equation a set of linear equations[3/9]. His approach is applicable to any differencing scheme of the transfer equation without regard to geometry or mesh size. However, equations in P_1 acceleration are algebraically difficult to solve. Hence efficiency remains a serious issue for higher dimensional problems. The approach we have taken to obtain the low order equation is the one proposed by Alcouffe[3/4] and later improved by Larsen[3/10].

The main objective of the DSA scheme is to synthesize a low order form for the radiative transfer equation, which can be used to accelerate the rate of convergence of the transfer equation. In addition, we require the new method to exhibit the following characteristics:

1. It offers a solution to the exact transfer equation, rather than just an approximation, such as the diffusion equation.
2. It is computationally efficient.
3. The method should be extendable to higher dimensions and to curvilinear geometry.
4. One should be able to solve more complicated problems, such as problems involving scattering.

From our experience we are able to prove the first two characteristics of the method, proof for the later two is beyond the scope of the present research; however, it has been reported[3/11,12] that these can also be satisfied.

3.5.2 DIFFUSION SYNTHETIC ACCELERATION:

A Fourier stability analysis of the transfer equation (presented in section A.1 of the appendix) shows that the most slowly converging modes (correspond to $\lambda \approx 0$) are given as

$$D(\lambda,\nu,\mu) = \frac{\chi\eta}{2}\frac{1}{(\sigma+\tau)}\left(1-\frac{i\lambda\mu}{\sigma+\tau}+O(\lambda^2)\right)$$

(3.5.01)

This equation indicates that the slowly varying modes are linear function of μ. We

use this fact to derive an equation which replaces (3.4.02c) and the end result is a faster convergence of (3.4.02a). Physically, the slowest converging modes correspond to near equilibrium situations. Therefore, in a sense we can guess that the low order form will resemble a diffusion equation.

We will use equation (3.3.12) to illustrate the **DSA** formulation. Its discretized version is given in Appendix A.3, since its subtle differences are not trivial. The steps that are commonly used to obtain the low order form of the transfer equation are as follows:

i. The zeroth and first moments of (3.3.12) in angular space are taken, that is equation (3.3.12) is multiplied by the weight functions 1 and ω_m followed by an integration of the resultant equations over angular space.

ii. I_1 is eliminated from the above two equations.

iii. The accelerated form of the resultant equation in (ii) is obtained by resetting the index of iteration for the zeroth and first moments of the intensity (that is $l+1/2 \rightarrow l+1$ for I_o and I_1).

The final result is

$$-\frac{\partial}{\partial x}\frac{1}{3(\sigma+\tau)}\frac{\partial}{\partial x}I_0^{l+1} + (\sigma+\tau)I_0^{l+1} = \eta\chi\int_0^{\infty}\sigma I_0^l d\nu + Q_0 - \frac{\partial}{\partial x}\frac{1}{3(\sigma+\tau)}Q_1 + \frac{\partial}{\partial x}\frac{2}{3(\sigma+\tau)}\frac{\partial I_2^{l+1/2}}{\partial x} \qquad (3.5.02)$$

This is simply the diffusion equation corresponding to the transfer equation when I is linear in angle, since when I is linear in angle $I_2=0$. It is shown in the appendix (section A.2) that the spectral radius for (3.3.12) with (3.5.02) goes to zero even for those modes for which (3.3.12) with (3.4.02) has spectral radius close to unity. This **apparently** seems to have **solved our problem**, but we will see this is not so. In equation (3.5.02) the right hand side contains a coupling term; therefore, we will have to solve this equation using source iteration, as was done for the radiative transfer equation.

3.6 GREY DIFFUSION EQUATION:

A Fourier stability analysis of (3.5.02) with source iteration shows that the spectral radius can be very close to unity. Therefore, to significantly improve the convergence rate of the transfer equation (3.3.12) we must improve the spectral radius of the diffusion equation (3.5.02) by another low order equation or by some other approximation. To accelerate the rate of convergence of the diffusion equation we choose to solve a low order form of diffusion equation, namely the grey diffusion equation, to obtain the new source term for the diffusion equation.

First of all we rewrite (3.5.02) as

$$-\frac{1}{3(\sigma+\tau)}\frac{\partial^2}{\partial x^2}I_0^{k+\frac{1}{2}} + (\sigma+\tau)I_0^{k+\frac{1}{2}} = \eta\chi\int_0^{\infty}\sigma I_0^k d\nu + S \qquad (3.6.01)$$

where S includes all the terms that do not change during the iteration of the diffusion equation. In the source iteration method we take

$$I^{k+1} = I^{k+1/2} \qquad (3.6.02)$$

A Fourier stability analysis of (3.6;01,02) shows that the diffusion equation can have a radius of convergence that is close to unity. If for simplicity we assume that the opacity is spatially independent in the Fourier stability analysis, then the radius of convergence and the corresponding eigen function are given by

$$\omega = \eta\int_0^{\infty}\frac{3\sigma(\sigma+\tau)\chi}{\lambda^2+3(\sigma+\tau)^2}\,d\nu \qquad \Psi = \eta\frac{3\sigma(\sigma+\tau)\chi}{\lambda^2+3(\sigma+\tau)^2}\,e^{i\lambda x} \qquad (3.6.03a,b)$$

This also shows that the slowest converging modes correspond to modes that are close to equilibrium modes. In order to accelerate the diffusion equation, we solve it by using the synthetic approach. That is, we use a grey equation as the low order equation.

The central idea behind the grey equation is to collapse the continuous energy

dependence in (3.6.01) to one energy group and design this equation such that the near equilibrium situation is treated more accurately than in the source iteration method. This new equation replaces (3.6.02). The steps involved in the derivation of the grey equation are as follows:

i. The first term in equation (3.6.01) is approximated by

$$-\frac{1}{3(\sigma+\tau)}\frac{\partial^2}{\partial x^2}I_o^{k+\frac{1}{2}} = -\frac{1}{3(\sigma+\tau)}\frac{\partial^2}{\partial x^2}\varphi^{k+\frac{1}{2}}\hat{I}_o^{k+1} + \frac{1}{3(\sigma+\tau)}\frac{\partial^2}{\partial x^2}\varphi^{k+\frac{1}{2}}\hat{I}_o^{k+\frac{1}{2}} - \frac{1}{3(\sigma+\tau)}\frac{\partial^2}{\partial x^2}I_o^{k+\frac{1}{2}}$$

and

$$I_o^k \text{ or } I_o^{k+\frac{1}{2}} = \theta^{k+\frac{1}{2}}\hat{I}_o^{k+1} - \theta^{k+\frac{1}{2}}\hat{I}_o^{k+\frac{1}{2}} + I_o^{k+\frac{1}{2}}$$

$$\hat{I}_o^{k+\frac{1}{2}} = \int_o^\infty \sigma I^{k+\frac{1}{2}}\,d\nu$$

(3.6.04)

An important characteristic of this transformation is that it ensures that after convergence, the left side of (3.6.04) is the same as the right side, implying that the converged solution for the source and the accelerated equation are the same. Variables θ and φ will be explained later.

ii. Integrate (3.6.01) over the frequency spectrum.

The final result is

$$-\int_0^\infty \left[\frac{1}{3(\sigma+\tau)}\frac{\partial^2}{\partial x^2}\varphi^{k+\frac{1}{2}}\right]d\nu\; I_0^{k+1} + (\sigma+\tau)I_0^{k+1} + \tau\left(\int_0^\infty \theta^{k+\frac{1}{2}}d\nu\right)I_0^{k+1}$$
$$= \eta I_0^{k+1} + \int_0^\infty S\,d\nu + \int_0^\infty \left[\frac{1}{3(\sigma+\tau)}\frac{\partial^2}{\partial x^2}\left(I_0^{k+\frac{1}{2}} - \varphi^{k+\frac{1}{2}}I_0^{k+\frac{1}{2}}\right)\right]d\nu$$
$$\tau\int_0^\infty \left[I_0^{k+\frac{1}{2}} - \theta^{k+\frac{1}{2}}I_0^{k+\frac{1}{2}}\right]d\nu - \eta I_0^{k+\frac{1}{2}} + \eta\int_0^\infty \sigma I_0^{k+\frac{1}{2}}\,d\nu$$

(3.6.05)

$\theta^{k+1/2}$ and $\varphi^{k+1/2}$ are defined[3/13] such that above equation produces an exact solution without iteration when I_o corresponds to the slowest converging modes. From (3.6.03) we see that the eigenvalue and the eigenfunction corresponding to the

slowest modes are

$$\omega = \eta \int_0^{\infty} \frac{\sigma\chi}{(\sigma+\tau)}\, d\nu \qquad \Psi = \eta \frac{\chi}{(\sigma+\tau)}\, e^{ikx}$$

(3.6.06)

We take the spectral functions (in normalized form) to be

$$\theta^{k+\frac{1}{2}} = \varphi^{k+\frac{1}{2}} = \frac{\dfrac{\chi}{(\sigma+\tau)}}{\left(\int_0^{\infty} \dfrac{\sigma\chi}{(\sigma+\tau)} d\nu\right)}$$

(3.6.07)

This choice of spectral function produces the linear grey equation. It is called linear because it leads to an additive correction. The other expressions for θ and φ are given by

$$\theta^{k+\frac{1}{2}} = \frac{I_o^{k+\frac{1}{2}}}{\hat{I}_o^{k+\frac{1}{2}}} \qquad ; \qquad \varphi^{k+\frac{1}{2}} = \frac{\left(\dfrac{\partial I_o^{k+\frac{1}{2}}}{\partial x}\right)}{\left(\dfrac{\partial \hat{I}_o^{k+\frac{1}{2}}}{\partial x}\right)}$$

(3.6.08)

Here the correction term is multiplicative, hence it is nonlinear. The main difference between these methods lies in the approximation to the grey spectrum. In the linear case we take it to be the spectrum corresponding to equilibrium, while in the nonlinear case it is the latest spectrum averaged coefficient. This can be rephrased as follows: the linear case grey method is defined by collapsing the cell average flux as the spectral function, while in the nonlinear grey case it is the cell edge flux that is collapsed as the spectral function.

The solution to the radiative transfer equation involves solving the following set of equations (3.3.12), (3.5.02) and (3.6.05). Equation (3.3.12) is solved first, then equation (3.5.02) and (3.6.05) are solved. This form of iteration can be viewed as

inner and outer iteration In the inner iteration equations (3.6.05) and (3.5.02) are repeatedly solved until (3.5.02) is converged. Then equations (3.5.02) and (3.3.12) are solved until (3.3.12) is converged to the desired accuracy. When the above equations are discretized, the consistency in the discretization of the equations and their boundary conditions is crucial for a physically acceptable and stable solution. This is addressed in Appendix (A.4).

CHAPTER FOUR
MODEL PROBLEM

The numerical aspects of the technique used to solve the radiative transfer equation are presented in Chapter Three. In this chapter, results are presented for the model problem that is used to test the present code. This chapter also includes a discussion of the issues which often arise with any code - issues such as fixups, stability, efficiency and the validity of the code. A comparison of the source iteration (SI) method and the diffusion synthetic acceleration (DSA) method is presented in this chapter. It will be shown later that when the DSA method is stable, it is always faster than the SI method and yields the same results. The extent to which DSA improves the spectral radius depends on different parameters, such as the time step, convergence criterion and the number of inner/outer iterations.

4.1 FIXUPS AND THE STABILITY OF THE CODE:

It often becomes necessary to incorporate fixups into codes that involve complicated equations and the DSA method is no exception. The main objective of these fixups is to suppress the appearance of nonphysical results. For example, the intensity is a physical quantity which can not be allowed to have a negative value. Therefore, it is important that some fixup should be implemented when negative intensity leads to instability.

The fixups are based on the trial and error approach and hence do not have any real theoretical justification, other than that they prevent nonphysical results from appearing in the simulations. Their presence in the code does not imply that they are used in every simulation. The important rule we have learned for a fixup strategy is that a fixup should be invoked only when the solution has become unstable not because it is becoming unstable. Every effort should be made to ensure

that the transfer equation, the diffusion equation and the grey equation are consistent at all times. A negative value may be physically unacceptable, but mathematically a negative value is as good as a positive value. Hence a negative value should not be modified unless a physically unacceptable solution is obtained or the code has become unstable. In this section we discuss some of the fixups implemented in the code.

The first fixup that is implemented is due to the spatial differencing scheme employed in differencing the radiative transfer equation in space. The Diamond differencing scheme is used to discretize the transfer equation in space, because of the ease of its implementation. Unfortunately, it can lead to a negative specific intensity, which if not corrected can destabilize the code. When a cell edge intensity becomes negative, it is taken to be zero or is set to be the average intensity of the cell. The choice depends on a parameter which is a function of the cell width and the time step (section A.3). Another important fixup which also has been included in our theoretical analysis is the incorporation of the above fixup into the diffusion equation. The Diamond Difference relationship in the diffusion equation is redefined as

$$I_{ogi}^{l+1}=\frac{1}{2}[a_{ogi}I_{ogi-\frac{1}{2}}^{l+1}+b_{ogi}I_{ogi+\frac{1}{2}}^{l+1}]$$

When a fixup is required in the transfer equation, the coefficients a_{ogi} and b_{ogi} are given as

$$a_{ogi}=\frac{I_{ogi}^{l+\frac{1}{2}}}{I_{ogi-\frac{1}{2}}^{l+\frac{1}{2}}} \quad , \quad b_{ogi}=\frac{I_{ogi}^{l+\frac{1}{2}}}{I_{ogi+\frac{1}{2}}^{l+\frac{1}{2}}}$$

Without the fixup, these coefficients are

$$a_{ogi}=b_{ogi}=1.0$$

(4.1.01a,b,c)

The choice of these coefficients depends upon the stability of the solution rather than on some theoretical analysis. The main objective is to define these coefficients so that the diffusion matrix yields a stable solution. From equation (A.8.02), we see that the main diagonal element is not always the dominant element. This can lead to a negative solution of the diffusion equation. If a negative solution of the diffusion equation occurs too frequently, the solution for the transfer equation may become unstable or become physically unacceptable. This problem can be eliminated through the use of small time steps so that the gradient opacity is small. One can also modify the algorithm[4/1] to ensure that the main diagonal element is always dominant, but this modification leads so slower acceleration of the diffusion equation.

In simulations it was observed that when the negative flux fixup is implemented, $I_{ogi\pm1/2}$ can become zero causing a floating point error in (4.1.01b) when a_{ogi} and b_{ogi} are computed. In order to prevent a floating point error, we take $a_{ogi}=b_{ogi}=1.0$ whenever $I_{ogi\pm1/2}$ is zero.

Many switches are added into the code to ensure its stability and to prevent the code from consuming an excessive amount of time on iterations which are extremely slow to converge or start to diverge. If the diffusion equation yields a spectral radius greater than or close to 1.0, then the code automatically resorts to SI for that iteration when switch AUTACC=1. If it occurs too often, then the calculation is terminated. A similar type of switch is included to prevent the grey equation from yielding an unrealistic solution. If the solution of the diffusion or the grey equation becomes unstable too often then the calculation is again terminated. In the event that the integration is not achieved within the required precision or the resultant matrix is ill behaved, then the program is again terminated. The code has been written such that the error messages are written into a file named "analysis" for instabilities which do not cause termination. Error messages appear on the screen for those instabilities which require user input to continue or that require termination of the code. These switches improve the efficiency of the code but do not ensure DSA stability when large time step is used, as was expected in the beginning of the

study.

4.2 THEORETICAL ASPECTS OF THE MODEL PROBLEM:

Often a code is tested against a bench mark problem, before it is used to simulate real problems. The problem we use to test the code is the well known Marshak Wave bench mark[4/2]. This is the same model problem used by Alcouffe et al[4/3] and Velarde et al[4/4] to test their codes. Here a strong source (acting as a laser beam) is placed at one end of the plasma. The temperature (which is changing due to the propagation of the radiation) is computed as a function of space and time. In this section the equations involved in the formulation of the model problem are presented.

We start our formulation from equations (3.3.01;02;3a) derived in Chapter Three. These equation are repeated here for convenience

$$\frac{1}{c}\frac{\partial I}{\partial t}(x,\mu,\nu,t) + \mu\frac{\partial I}{\partial x}(x,\mu,\nu,t) + \sigma(\nu,T)I(x,\mu,\nu,t) = S(\nu,T) = \sigma(\nu,T)B(\nu,T)$$

$$\frac{\partial u_s(T)}{\partial t} = \beta(T)\left[\int_0^\infty \sigma(\dot{\nu},T)I_0(x,\dot{\nu},t)d\dot{\nu} - c\sigma_p(T)u_s(T) + S_{ext}\right]$$

$$u_s(T) = \frac{c}{4\pi}\int_0^\infty B(T,\dot{\nu})\,d\dot{\nu}$$

(4.2.01;02;03)

For the model problem, we assume that a local thermodynamic equilibrium (LTE) exists in the plasma. In LTE, it is assumed that properties of the matter are dominated by atomic collisions which establish thermodynamic equilibrium locally at a position x and at time t, and that the radiation field does not affect this equilibrium even when it deviates substantially from the Planckian distribution. That is, at a given instant of time and point in space it is sufficient to specify two thermodynamic quantities, such as the temperature and density in order to compute the source term S($=\sigma$B) and the absorption coefficient σ. With the LTE assumption, B becomes the Planckian function and the transfer equation reduces to

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu\frac{\partial I}{\partial x} = \sigma(B - I)$$

$$\frac{\partial u_s}{\partial t} = \beta\left[\int_0^\infty \int_{-1}^{1} \sigma I \, d\mu d\nu - c\sigma_p u_s\right]$$

$$u_s = \frac{c}{4\pi}\int_0^\infty B \, d\nu = aT^4$$

(4.2.04;05;06)

where σ and B are defined as

$$\sigma = a_1\frac{[1-e^{-a_0\nu}]}{\nu^3} \qquad B = \frac{2h\nu^3}{c^2}[e^{a_0\nu} - 1]^{-1}$$

$$\textit{where} \quad a_0 = \frac{h}{KT} \quad \textit{and} \quad a_1 = 3.8171E55 \ m^{-1}$$

(4.2.07)

where T is the material temperature, a (=7.560667E-16 $Jm^{-3}K^{-4}$) is the Stefan Boltzmann constant, h (=6.626E-34 Js) is the Planckian constant, k (1.3807E-23 JK^{-1}) is the Boltzmann constant. When equation (4.2.04) is discretized in frequency (Chapter Three) it reduces to

$$\mu\frac{\partial I_g}{\partial x} + (\sigma_g + \tau)I_g = \frac{\chi_g \eta}{2}\Sigma_g \, \sigma_g I_{0g} + Q_g$$

(4.2.08)

For the model problem, the initial intensity in the summation term on the right hand side of the above equation is taken to be Planckian and the absorption coefficient is computed as

$$\sigma_g = \frac{\int_{\nu_l}^{\nu_h} \sigma\omega \, d\nu}{\int_{\nu_l}^{\nu_h} \omega \, d\nu}$$

(4.2.09)

where $\omega(\upsilon)$ is the weight function corresponding to the intensity at that moment. Since this is unknown an approximation is usually made. The choice of this function

is somewhat arbitrary. The weight functions which we have included in the code are known as Planckian and Rossland Mean functions. These functions are given by[4/5]

$$\omega(\nu) = B(\nu) \qquad \textit{Planckian}$$
$$\omega(\nu) = \frac{1}{\sigma(\nu)} \frac{\partial B(\nu)}{\partial T} \qquad \textit{Rossland}$$

(4.2.10a,b)

Their justification is based on the following argument[4/5]. The Planckian function B is a good approximation at thermodynamic equilibrium since the specific intensity is given by a Planckian function, and away from equilibrium the choice of the weight function is of less importance. The Rossland function is a good approximation since the specific intensity can be approximated by the equilibrium diffusion approximation. The choice of these functions becomes less significant if a large number of frequency groups are used.

The Romberg integration approach is used to integrate these functions. Lower-Upper decomposition is implemented to invert the matrices in both the diffusion and the grey equations.

4.3 SIMULATIONS OF THE MODEL PROBLEM:

The main objectives of this section are to test the code against a bench mark problem and make comparison between the two approaches used to solve the transfer equation, namely the Source Iteration (SI) and Diffusion Synthetic Acceleration (DSA) methods. The SI method always yields a stable solution irrespective of the time step involved. The DSA becomes unstable for large time steps, but when it works, it is more efficient than SI and yields the same results as the SI methods.

The model problem we used to test the code involves a slab at uniform temperature with a source at one end. The source is placed at the left boundary and it is assumed to be Planckian. This choice for a source resembles a laser beam incident on a foil. It is assumed that the specific heat of the plasma is constant

during the simulation, that is it is independent of the temperature. The convergence criterion is set to be

$$[\frac{I^{n+1}}{I^n} - 1] \leq 10^{-2} \qquad [\frac{T^{n+1}}{T^n} - 1] \leq 10^{-3}$$

This simply states that the specific intensity of the transfer equation is considered to have been converged when the error between two consecutive solutions is less than 1%. A similar convergence criterion is used for the temperature but a convergence criteria of 0.1% is used instead of 1.0%. If the time step is large (such as in nano seconds) then tighter convergence is essential. Once the intensity has converged we use the so called "parametric iteration" to update the temperature. In parametric iteration we use the new temperature (obtained after solving the energy balance equation) to compute the variables (such as σ and χ) that should have been computed at the advanced time step. This is repeated until the temperature is converged to the desired accuracy. The data set used for the standard model problem is

number of cells (uniform)	20
number of frequency groups	30
number of discretized angles	08
specific heat per unit volume	7.00E+04 $JK^{-1}m^{-3}$
source temperature	1000 ev
initial slab temperature	1 ev
slab width	0.2 m
frequency range	1.00E-01-1.00E+04 ev

Additional parameters will be mentioned when appropriate.

Many runs were made to explore the performance of the DSA method. In the remainder of this section, we will discuss important aspects related to the efficiency of the code. We have observed that when very small time steps are used (e.g fraction of a picosecond) the DSA method is not very efficient compared to the SI method. When time steps are small, it is more efficient to use the Source Iteration

method, because the time taken to solve the diffusion and grey equation out weighs the efficiency of the DSA method over the SI method. The efficiency of the DSA method improves as we increase the time step. In our simulations, the maximum time step allowed for a stable DSA solution is about 100.0 picoseconds for the model problem. The efficiency of DSA relative to SI depends on the convergence criteria. A tighter convergence criteria with the DSA method results in a small increase in computer time but it significantly increases with the SI method. It is observed that if the number of inner iterations (number of diffusion equations per transfer equation) is not bounded, then not only the efficiency drops but also this can destabilize the code. It is observed that if inner iterations are bounded by 10 then DSA is more efficient and stable compared to when the number of inner iterations is allowed to be unlimited. The solution of the diffusion equation without the grey equation very often increases the computer time for a given simulation (even though it improves the spectral radius) due to slow convergence rate of the SI. However, the time is substantially reduced when the diffusion equation is solved using the grey equation.

Therefore, in order to optimize the efficiency of the code, it is important that the diffusion equation is solved with the grey equation and that a bound is placed on the inner iterations. The remainder of this section includes a graphical representation and a discussion of the following topics:

i. A comparison between DSA and SI .

ii. Planckian vs Rossland weight functions.

iii. Use of exponential temperature as the initial temperature (instead of being uniform).

iv. Effect of varying the number of cells, number of frequency groups and number of discretized angles.

v. Marshak Wave Bench Mark

The source code is in a file name **"sate.f"** (a listing can be found in the appendix) and the input file is called **"sate.data"** and is given below.

satedata

ENTER 1 FOR RUNS WITH DIFFERENT TIME STEPS OTHERWISE 0	00
ENTER SCR NUM DBXL DBXU TCONT	00 02 0000 9999 01
ENTER T OR F FOR SIMULATIONS OF THE MODEL PROBLEM (SIMRUN)	F
ENTER "0" IF SOURCE IS TO BE DEPENDENT ON TIME (TEMPTD)	01
ENTER "0" IF INITIAL TEMPERATURE DISTRIBUTION IS EXP (TEMEXP)	01
ENTER "0" IF ALWAYS USE NFF (NFMUST)	01
ENTER "0 TO 20" FOR OUTPUT TO BE PRINTED (PRES)	00
ENTER BOUND FOR TRANSPORT AND DIFFUSION EQU (TB DB)	9999 999
ENTER "0" IF (INTB=0) "1" IF (INTB=PINB) "2" IF USE MTSP (NFFC)	02
ENTER IERR AND TERR AND SIER	1.00E-02 2.50E-01 1.00E-02
ENTER # OF OIT AFTER WHICH NEGATIVE FLUX IS ALWAYS USED (INSB)	999999
ENTER ABSORPTION COEFFICIENT 1E? (? = 6 TO 11) (AC)	1.00E+11
ENTER "0 TO 2" FOR CONVERGENCE CRITERION BEST IS "1" (CONVC)	01
ENTER "0" IF INITIAL INTENSITY TO BE PLANCKIAN EACH TIME (TRIN)	01
ENTER "0" IF UNIFORM SPATIAL DISTRIBUTION IS TO BE USED (USC)	00
ENTER TIME INTERVAL AT WHICH TEMPERATURE IS TO SAVED (PRTME)	1.00E-09
ENTER "0 OR 1" DIFFUSION BC (DIFBC)	00
ENTER "0 TO 2" TO OVERCOME NEGATIVE DIFFUSION INTENSITY (NDIT)	03
ENTER MAXIMUM TIME FOR SIMULATION (MAXT)	1.01E-07
ENTER M < 9 G < 61 N < 151	008 030 020
ENTER L LFL UFL TELB ITRB ITSL 2.00E-01 1.00E+01 1.00E+03 2.00E-02 1.00E+01 1.00E-00	
ENTER "0" IF PLANCKIAN IS TO BE USED AS A WEIGHT (WFN)	00
ENTER SPECIFIC HEAT (SPH)	7.00E+04
ENTER DTIME	1.00E-12
ENTER "0" IF NEGATIVE FLUX FIX UP IS TO BE IMPLEMENTED (NF)	00
ENTER NUMBER OF TEMPERATURE ITERATIONS ALLOWED (TITA)	9999
ENTER NUMBER OF OUTER ITERATIONS ALLOWED (OITA)	999992
ENTER "0" FOR LOWER LIMITS OTHERWISE "1" (SETLIM)	00
ENTER "0" FOR SOURCE = 0 AT RIGHT "1" FOR BOTH ENDS (SETSOU)	02
ENTER "1" IF NEG. FLUX TAKEN IT'S ABSOLUTE VALUE (ABVL)	00
ENTER "1" IF CODE TO BE EXECUTED WITH MEDUSA (MEDUSA)	01
ENTER "1" IF ACCELERATION IS AUTOMATIC (AUTACL)	00 5.00E-01
ENTER "0" IF TRANSPORT EQUATION IS TO BE SOLVED BY SI (TRNACC)	00
ENTER "1" IF DIFFUSION EQUATION IS TO BE ACCELERATED (DIFACC)	02
ENTER "0" FOR LINEAR GREY MODEL OR "1" FOR NONLINEAR (LIN)	00

Figure 4.1 a, b

When finer cells are used the computational time increases significantly, while the solution for the temperature remains very much the same. An increase in the temperature at the left end implies that the closer we move to the left (by making cells more finer), a higher temperature is obtained at the left end of the slab until it reaches the maximum value at the boundary (the value of the source). The difference in temperature can be reduced if a tighter temperature convergence criterion is used in both cases. A decrease in the number of cells has a more noticeable change in the temperature profile than when the number of cells is increased. The difference in the temperature with 50 cells compared to 20 cells (Fig. 4.1a) is relatively small while the computational time is significantly increased. The use of 10 cells (Fig. 4.1b) on the other hand shows a significant difference compared to 20 cells. Therefore, use of 20 cells is sufficient to yield an accurate description of the temperature in the slab for this case.

Figure 4.2 a, b

In the standard model problem 30 frequency groups are used. From Fig. 4.2a, it can be seen that increasing the number of frequency groups has no effect on the temperature profile that is observable. However, if the number of groups (Fig. 4.2b) is decreased then a significant change in the temperature profile is observed. Therefore, 30 frequency groups are sufficient in our simulations of the model problem.

Figure 4.3 a, b

Here it is shown that when the number of discretized angles is reduced (Fig. 4.3) then the entire temperature profile is shifted upward. We did not observe any significant significant change in the temperature profile (Fig. 4.3b) when number of discretized angles is increased to 16. Therefore, we think 8 discretized angles is sufficient to take into consideration the angular dependence of the intensity.

Figure 4.4

This graph represent the Marshak Wave Bench Mark with the present code. The profiles shown here are not exactly as reported by Alcouffe or Honrubia, this is because different weight function profiles are used for the absorption coefficient. This implies that the rate of change of temperature will be different; however we expect that the equilibrium profiles should be very much the same. This is true for all of the results reported by Alcouffe and Honrubia and reported here.

Figure 4.5

Here a comparison of SI and DSA is presented. This graph shows that the accelerated and non accelerated solution are the same. We have observed this consistency for all cases. In this graph a comparison between the linear and nonlinear grey models is also presented. We observed that the linear grey model performs better than the nonlinear model. The comparison of SI and DSA is shown below

	# of transfer equ.	# of diffusion equ	# parametric iteration
SI	1432	0	63
DSA(linear)	148	578	26
DSA(nonlinear)	148	1893	27

Our present code is not as stable as was expected. There appears to be a discrepancy in our derivation which we have not been able to resolve. The boundary conditions used for the grey equation in the code are the best in a sense that they yield the same result while allowing the use of a larger time step. The cause of this instability will require further investigation in the future. From our experience we think the inconsistency exists between the grey and the diffusion equation boundary conditions.

Figure 4.6 a, b

This graph reflects the effect of the weight functions used for evaluating the absorption coefficient. In Fig. 4.6a the number of groups is 30 and in Fig. 4.6b the

number of groups is 60. This shows that different choice of weight functions can lead to different temperature profiles. This graph also shows that as the number of groups is increased the choice of the weight function becomes less crucial. This conclusion is difficult to corroborate or disapprove because neither Alcouffe nor Honrubia has discussed the choice of the weight functions in their publications.

Figure 4.1 a

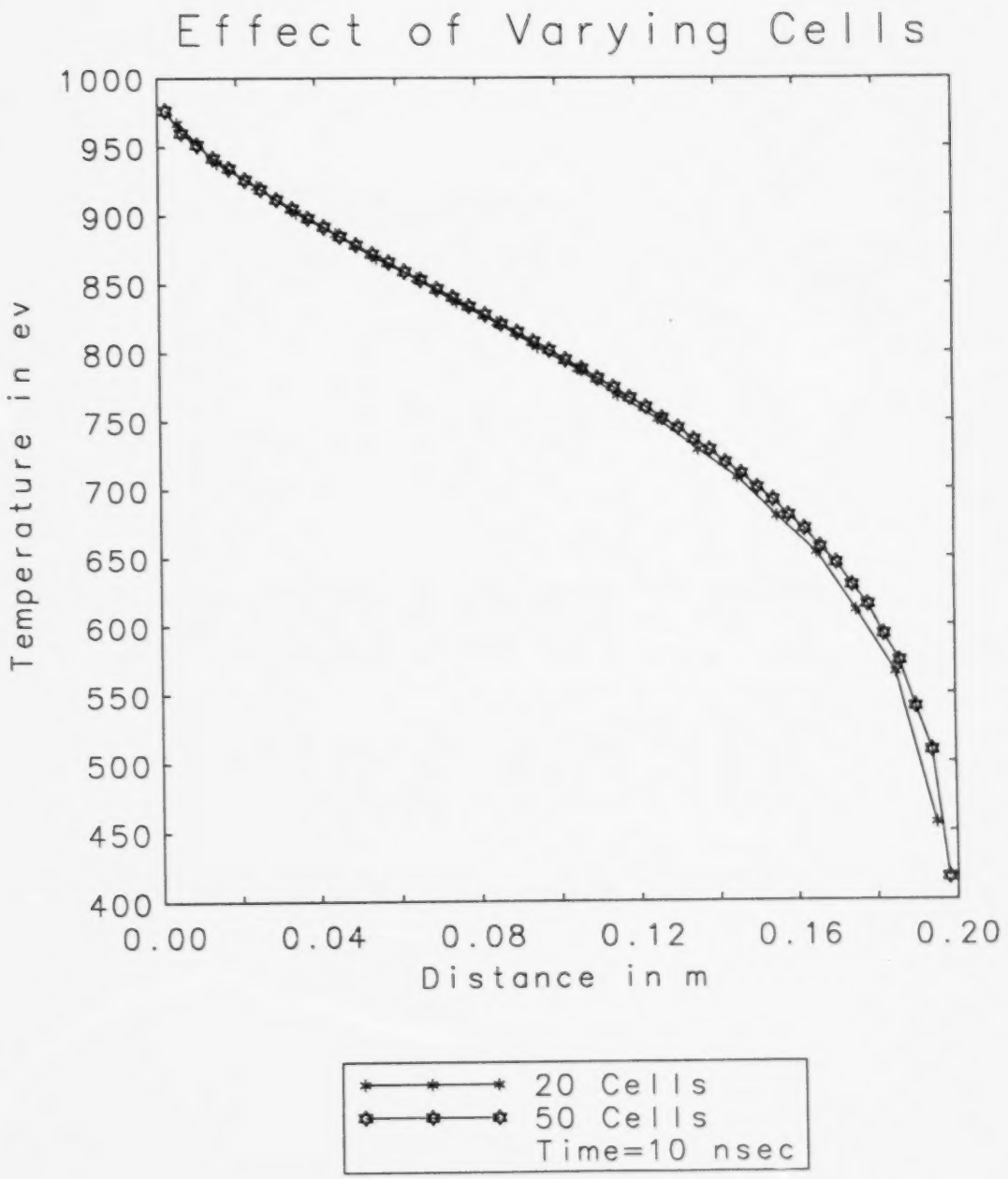

Effect of Varying Cells
Temperature in ev
1000
950
900
850
800
750
700
650
600
550
500
450
400
0.00
0.04
0.08
0.12
0.16
0.20
Distance in m
20 Cells
50 Cells
Time=10 nsec

Figure 4.1 b

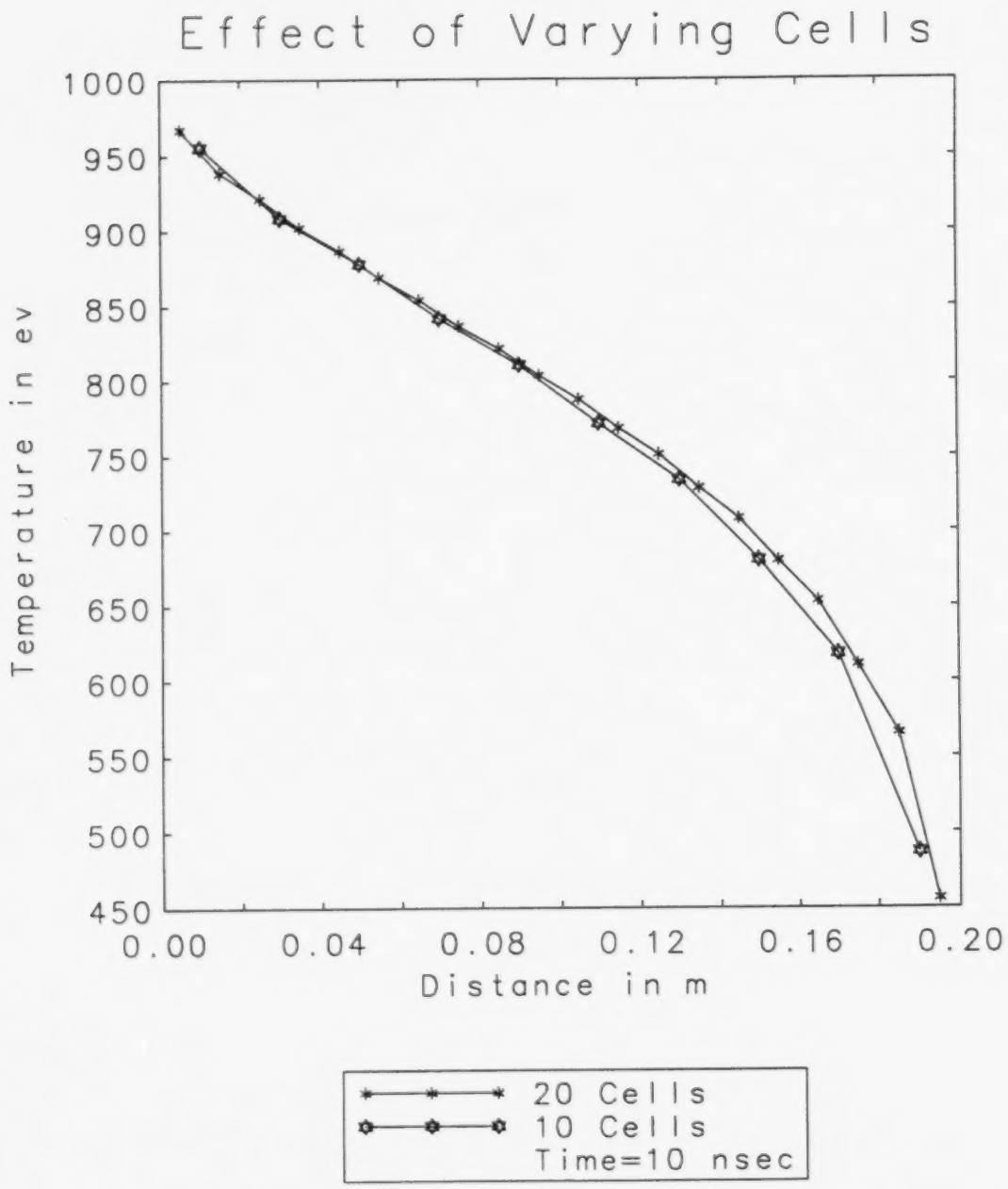

Effect of Varying Cells
Temperature in ev
1000
950
900
850
800
750
700
650
600
550
500
450
0.00
0.04
0.08
0.12
0.16
0.20
Distance in m
20 Cells
10 Cells
Time=10 nsec

Figure 4.2 a

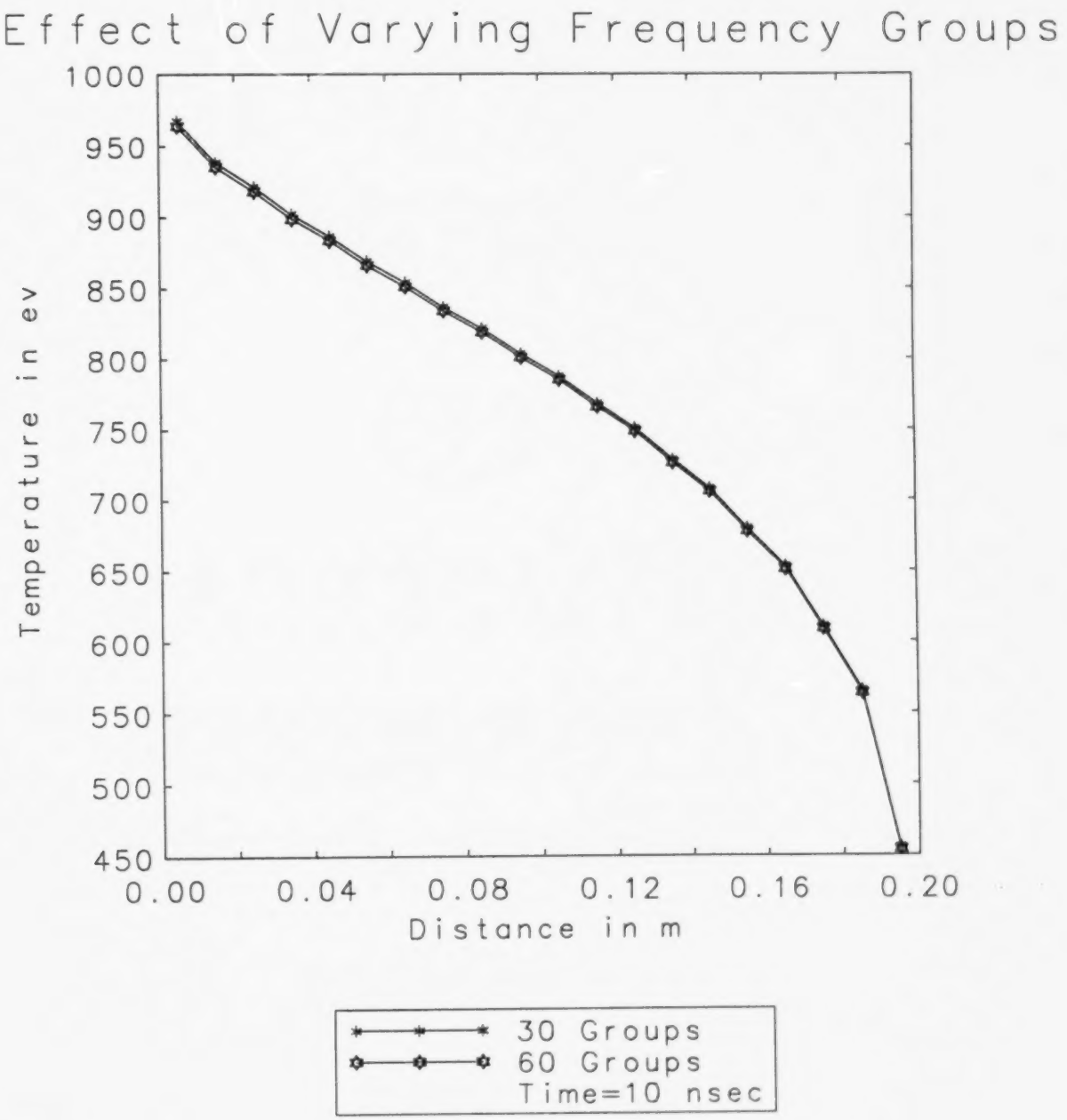

Effect of Varying Frequency Groups
Temperature in ev
1000
950
900
850
800
750
700
650
600
550
500
450
0.00
0.04
0.08
0.12
0.16
0.20
Distance in m
30 Groups
60 Groups
Time=10 nsec

Figure 4.2 b

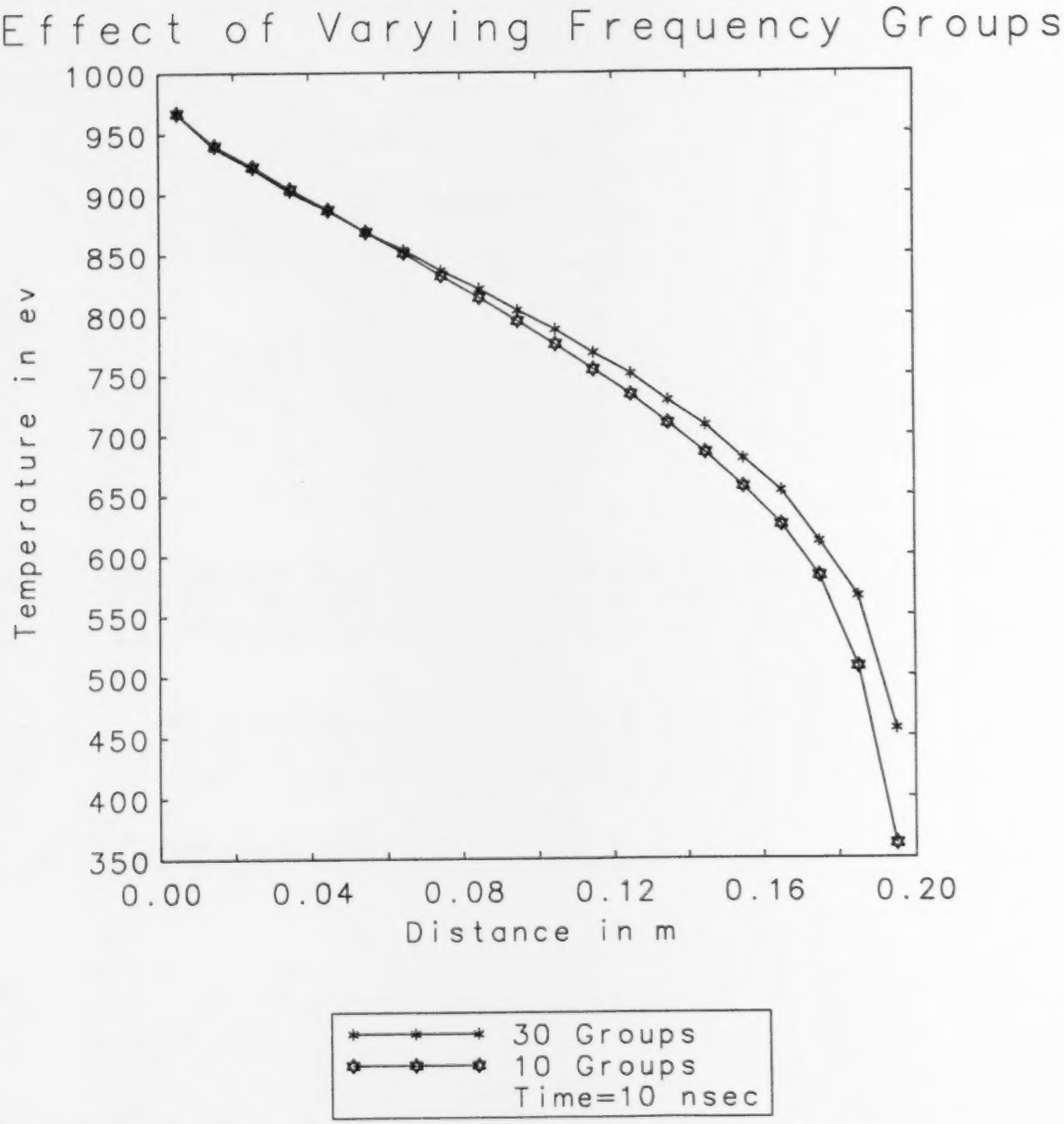

Effect of Varying Frequency Groups
Temperature in ev
1000
950
900
850
800
750
700
650
600
550
500
450
400
350
0.00
0.04
0.08
0.12
0.16
0.20
Distance in m
30 Groups
10 Groups
Time=10 nsec

Figure 4.3 a

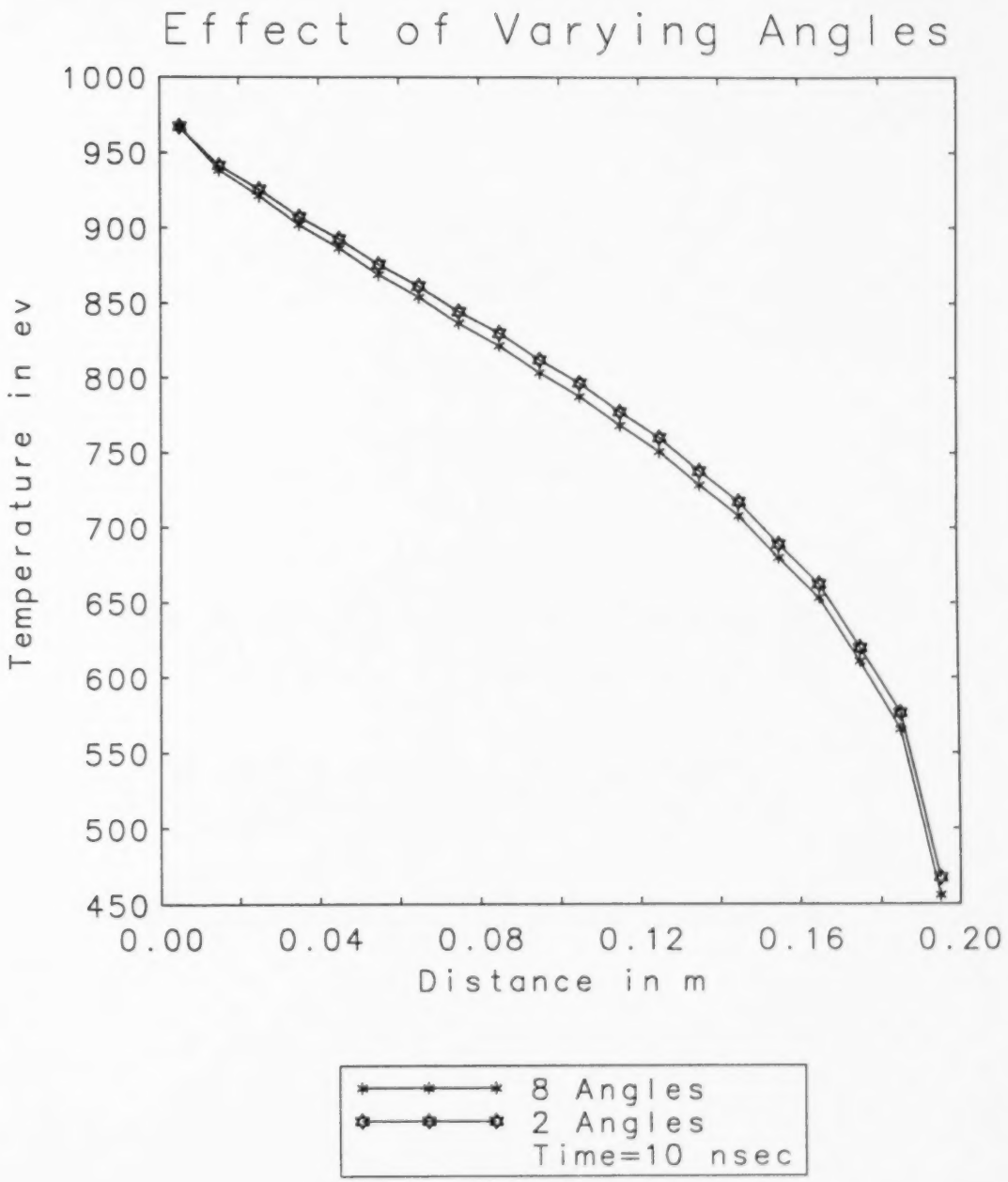

Effect of Varying Angles
Temperature in ev
1000
950
900
850
800
750
700
650
600
550
500
450
0.00
0.04
0.08
0.12
0.16
0.20
Distance in m
8 Angles
2 Angles
Time=10 nsec

Figure 4.3 b

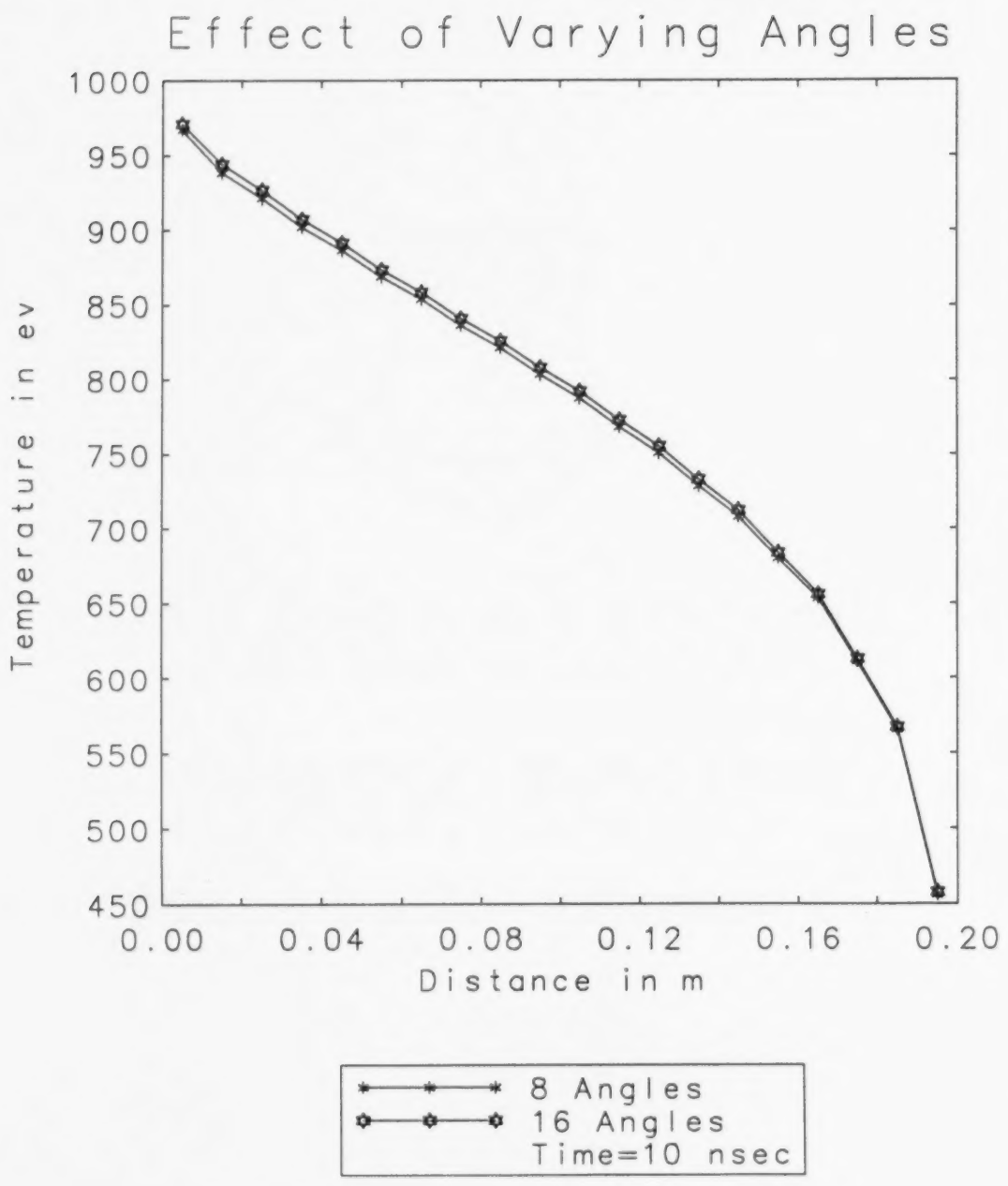

Effect of Varying Angles
Temperature in ev
1000
950
900
850
800
750
700
650
600
550
500
450
0.00
0.04
0.08
0.12
0.16
0.20
Distance in m
8 Angles
16 Angles
Time=10 nsec

Figure 4.4

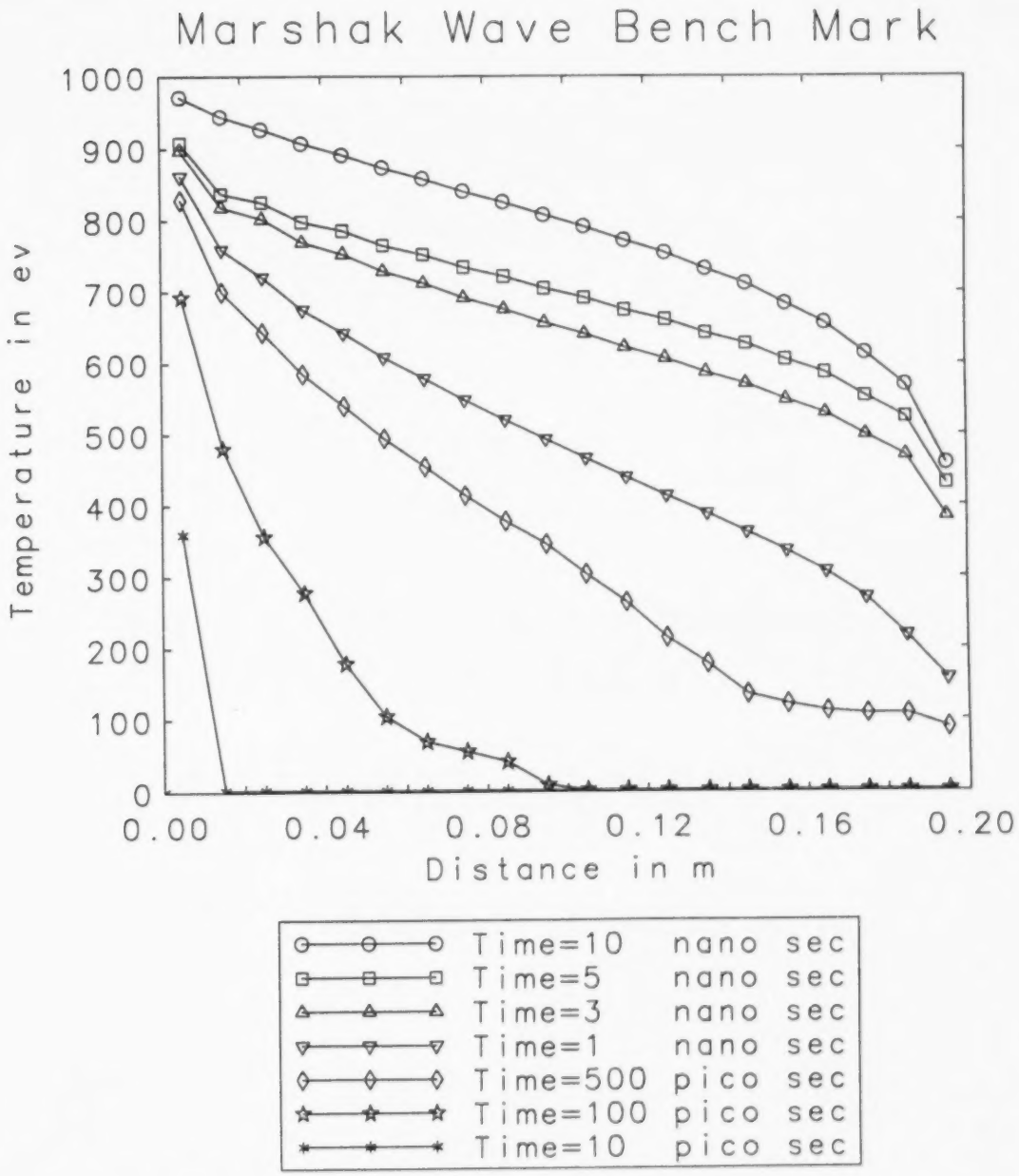

Marshak Wave Bench Mark
Temperature in ev
1000
900
800
700
600
500
400
300
200
100
0
0.00
0.04
0.08
0.12
0.16
0.20
Distance in m
Time=10 nano sec
Time=5 nano sec
Time=3 nano sec
Time=1 nano sec
Time=500 pico sec
Time=100 pico sec
Time=10 pico sec

Figure 4.5

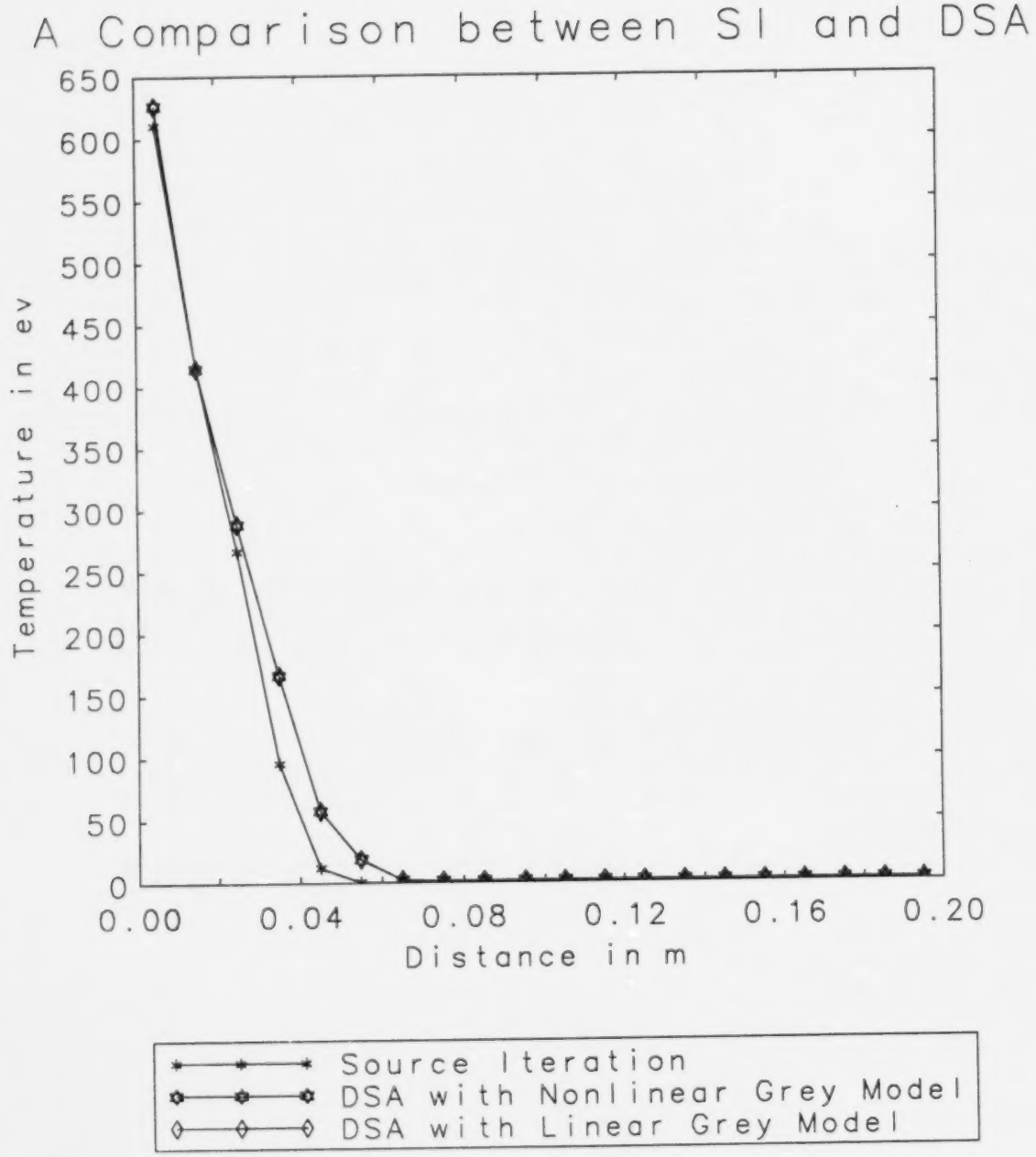

A Comparison between SI and DSA
Temperature in ev
650
600
550
500
450
400
350
300
250
200
150
100
50
0
0.00
0.04
0.08
0.12
0.16
0.20
Distance in m
Source Iteration
DSA with Nonlinear Grey Model
DSA with Linear Grey Model

Figure 4.6 a

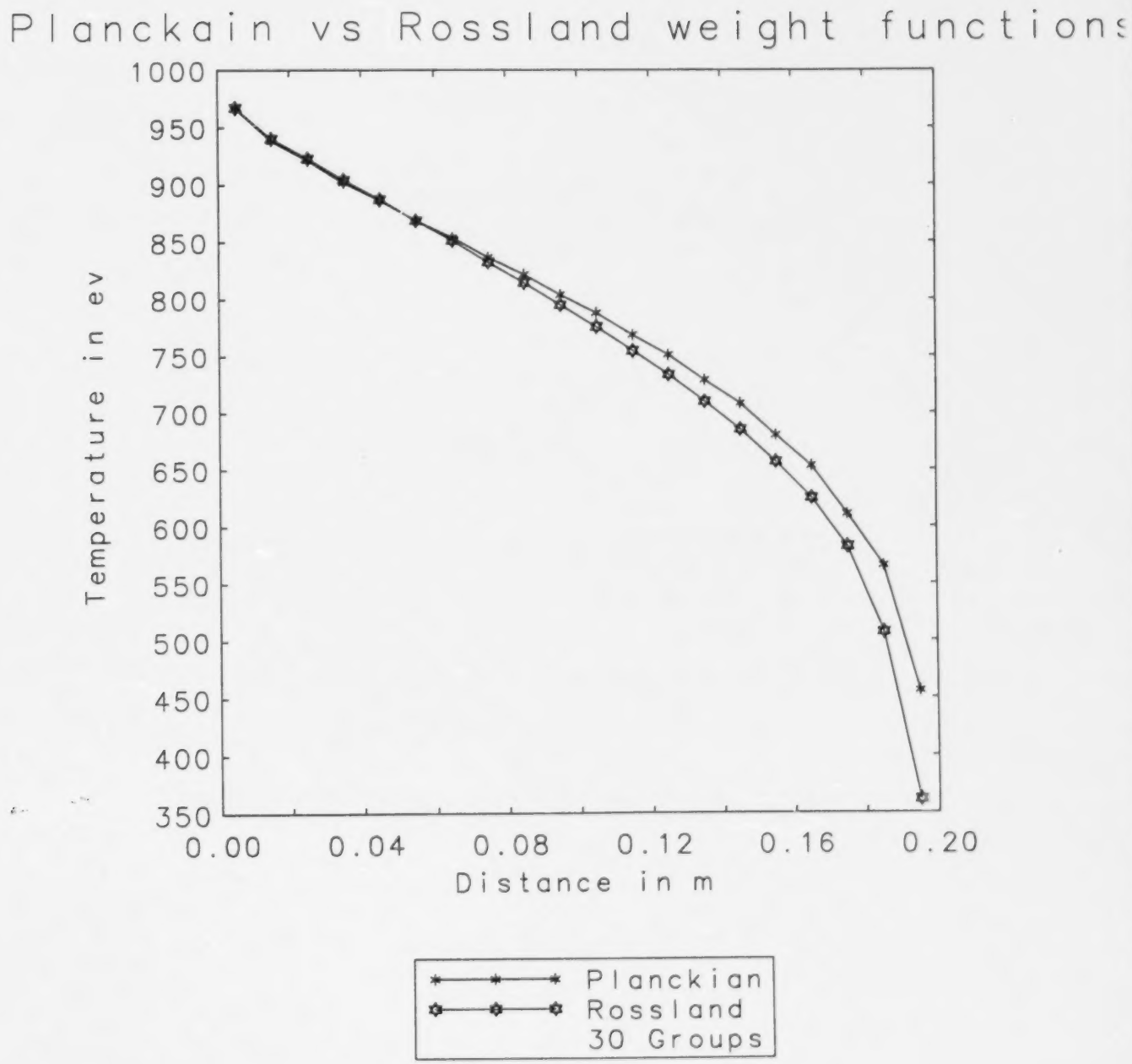
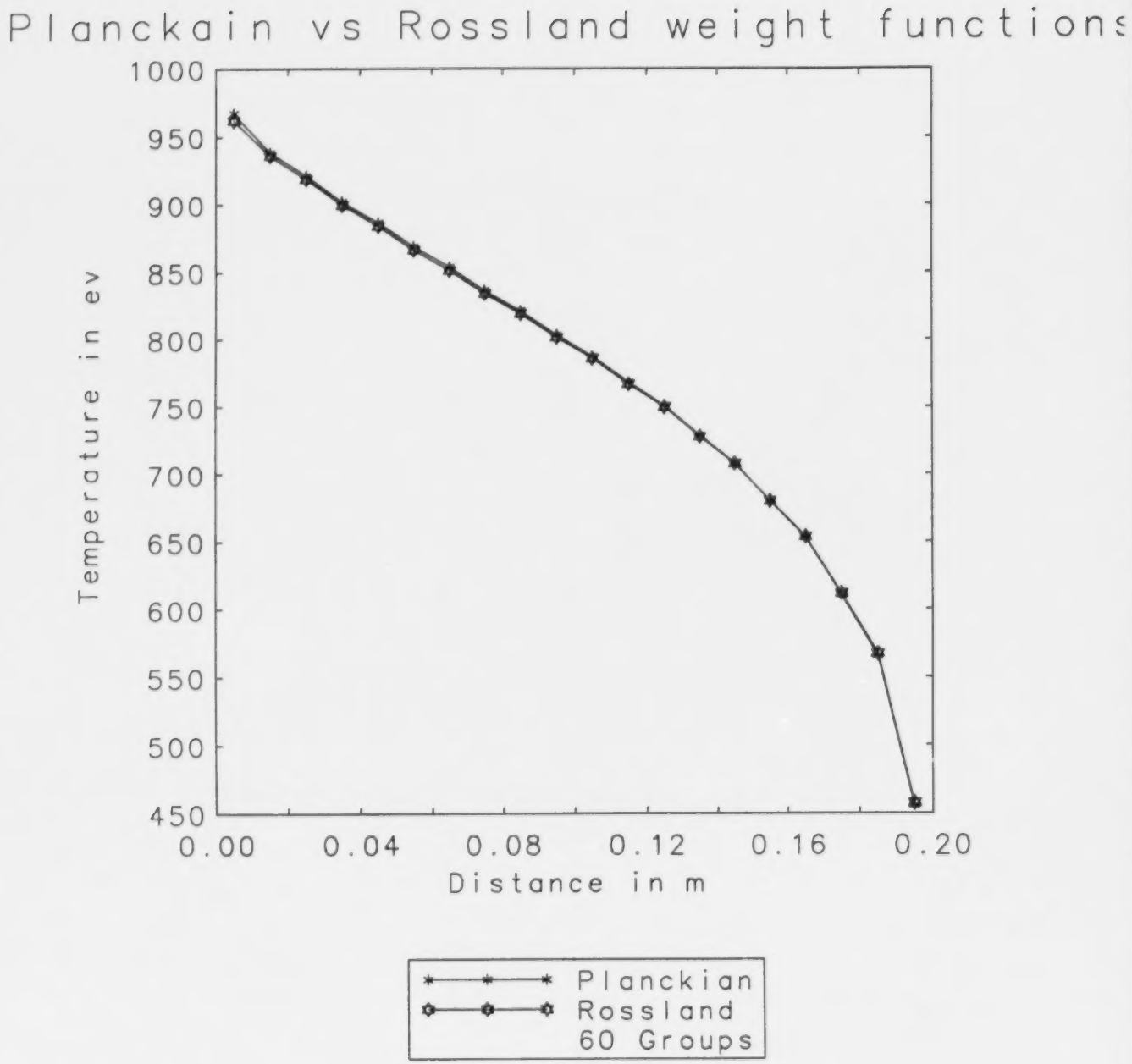

Planckain vs Rossland weight functions
Temperature in ev
1000
950
900
850
800
750
700
650
600
550
500
450
400
350
0.00
0.04
0.08
0.12
0.16
0.20
Distance in m
Planckian
Rossland
30 Groups

Figure 4.6 b


Planckain vs Rossland weight functions
Temperature in ev
1000
950
900
850
800
750
700
650
600
550
500
450
0.00
0.04
0.08
0.12
0.16
0.20
Distance in m
Planckian
Rossland
60 Groups

CHAPTER FIVE
MEDUSA SIMULATIONS

The objective of our research has been to study the nature and extent of the effects of radiation in laser produced plasma. We will show through simulations that the radiation plays an important role in the transport of heat in laser produced plasmas. The extent to which radiation affects the hydrodynamics of a plasma very much depends on the time profile and intensity of the laser beam to name few. An exclusion of radiative effects can lead to an erroneous estimate of radiation transported or loss of energy from a plasma. Although the inclusion of radiation transport into a hydrodynamic code is an arduous task, it is important because it gives a more accurate representation of the laser plasma interaction. This chapter has been divided into the following sections:

i. Introduction to MEDUSA

iii. Integration of the radiation code into MEDUSA

iii. Simulations using MEDUSA

This chapter will conclude the objective of our thesis. An extensive appendix is included at the end. The appendix includes the derivation of all of the equations used in the code **"sate.f"**.

5.1 INTRODUCTION TO MEDUSA:

In the mid 1970's a computer code named MEDUSA was written to simulate the laser fusion process. It was written for a one dimensional geometry in order to investigate the hydrodynamics and thermodynamics which take place in a small pellet. MEDUSA was refined later to accurately describe the interaction of laser light with a plasma. The MEDUSA code in its present form differs from the original due to modifications and additions made to it at University of Alberta. The present

version of MEDUSA gives a more realistic simulation compared to the original one. New features included are:

i. A modified equation of state, which is valid at low temperatures and near solid density.

ii. A simultaneous solution of electron and ion diffusion and equilibration equations.

iii. A calculation of the local ionization and x-ray emission from a radiative equilibrium model.

iv. Addition of the radiation transport.

In this section a brief summary of the equations solved by MEDUSA are outlined, more details can be found elsewhere[5/1].

5.1.1 PHYSICAL MODEL:

In MEDUSA, the plasma is assumed to consist of a charge-neutral mixture of electrons and various species of ions (a collective term for atoms, ions and molecules). Thermodynamically, the electrons and ions are treated as two subsystems, each with its own internal energy, temperature and pressure. The two subsystems are coupled via a common velocity which ensures neutrality of the mixture. The exchange of energy is due to electron-ion and electron-atom collisions. Electric fields are ignored. The instantaneous local chemical composition is described by a set of fractions f_k such that

$$n_k = f_k n_i$$

where f_k is subject to $\Sigma f_k = 1$, and n_k is the ion density of the kth species. The electron density changes with time due to hydrodynamic expansion and contraction of the moving fluid. The electron and ion densities are related by

$$n_i = n_e / Z \quad m^{-3}$$

where Z is the atomic charge of the matter. The physical density is given as

$$\rho = n_i M m_H \quad Kg\ m^{-3}$$

where M is the atomic mass (the electron mass is ignored), m_H is the hydrogen mass. The average mass and charge is calculated from

$$M = \Sigma f_k M_k \text{ and } \quad Z = \Sigma f_k Z_k$$

5.1.2 ENERGY EQUATION:

The energy equation is given as

$$C_v \frac{dT}{dt} + B_T \frac{d\rho}{dt} + P \frac{dV}{dt} = S \qquad Jkg^{-1}$$

where S is the rate per unit mass at which energy enters each system. This is given by the following expressions for electrons and ions

$$S_e = H_e + K + J + X + Y_e$$

$$S_i = H_i - K + Q + Y_i$$

where
- H: heat flow due to thermal conduction
- K: rate of energy exchange between the electron and ion fluids.
- J: rate of Bremsstrahlung emission
- X: rate of absorption of laser light
- Q: rate of viscous shock heating
- Y: rate of nuclear energy released (it is switched off in our simulations, since it is irrelevant to our research)

and P is the pressure and C_v and B_T are given as

$$C_v = \left(\frac{\partial U}{\partial T}\right)_\rho \qquad B_T = \left(\frac{\partial U}{\partial \rho}\right)_T$$

5.1.3 HEAT CONDUCTION:

The heat conduction is assumed to be classical and is given as

$$H = \frac{1}{\rho} \nabla \cdot \chi \nabla T$$

where the thermal conductivity χ for electrons and ions is

$$\chi_e = \frac{1.83E-10 T_e^{\frac{5}{2}}}{\log\Lambda Z \bar{Z}^2} \qquad W/m\ K$$

$$\chi_i = \frac{4.3E-12 T_i^{\frac{5}{2}}}{\log\Lambda \sqrt{M} Z^2 \bar{Z}^2} \qquad W/m\ K$$

$$\Lambda = \frac{1.24E06 T_e^{\frac{3}{2}} n_e}{\sqrt{n_e} Z}$$

where Λ is the coulomb logarithm.

5.1.4 ENERGY EXCHANGE:

The exchange of energy between electrons and ions occurs at the rate of

$$\omega = \frac{Z^2 e^4 n_i \log\Lambda \sqrt{m_e} (kT_e)^{\frac{3}{2}}}{M 32 \sqrt{2\pi} \epsilon_o^2 m_H} \qquad s^{-1}$$

the K term in the energy equation is

$$K = \frac{1}{\rho} \omega n_e k (T_i - T_e)$$

5.1.5 ENERGY EMITTED:

When radiation transport is not included, all of the radiation emitted from the plasma is taken to be via Bremsstrahlung emission by electrons and this emission is treated as a total loss. For a Maxwellian distribution it is given as

$$J = -8.5E-14 \frac{n_e \sqrt{T_e} \bar{Z}^2}{M} \qquad W K g^{-1}$$

5.1.6 ENERGY ABSORBED:

The absorption is assumed to occur via inverse Bremsstrahlung at a density ρ below critical density ρ_c, where ρ_c is given as

$$\rho_c = \frac{\epsilon_o M m_H m_e}{Ze^2}\omega_L^2$$

At $\rho = \rho_c$ the remaining power is deposited in the next adjacent cell and reflection of the laser intensity is neglected. The absorption coefficient is given as

$$\alpha = 13.51\beta^2 \frac{(5.05 + \log\lambda T_e)\bar{Z}^2}{\lambda^2\sqrt{1-\beta}\,T_e^{\frac{3}{2}}} \qquad m^{-1}$$

where β *is* $\qquad \beta = \frac{\rho}{\rho_c}$

If the initial laser intensity is P_o at $r = R_o$, then the power at r is given by

$$P = P_o e^{\alpha(R_o - r)}$$

5.1.7 MOTION OF THE PLASMA:

The motion of the plasma is governed by the Navier-Stokes equation

$$\rho\frac{du}{dt} = -\nabla P$$

where u is the velocity of the plasma and P is the total pressure, $P = P_i + P_e$.

5.1.8 EQUATION OF STATE:

The equation of state assumes that ions behave as a non-degenerate perfect gas, while electrons behave as being degenerate, non-degenerate or partially degenerate. The most recent EOS package gives a more accurate description of a metal at low temperatures and coincides with the EOS of the original MEDUSA at high temperatures. It is invoked by setting NLOM2(6)=.TRUE., NLOM2(7)=.TRUE. and STATE=-1 (for aluminum).

5.1.9 DIFFERENCING SCHEMES:

The cell edges are free to move, thereby altering the volume of the cell. The

quantities at the centre are obtained by averaging the values at the cell edges. A finite differencing scheme is used to discretize the equations shown above. The cell width varies such that the mass of the cell remains constant during the simulations, since thermonuclear burning is turned off.

5.1.10 TIME DIFFERENCING AND TIME STEP CONTROL:

MEDUSA uses a five level scheme. Levels 1,3,5 correspond to the time step n-1,n,n+1 respectively and levels 2,4 correspond to the time between n-1 & n and n & n+1. If we let r, ρ, $T_{e,i}$, to be the cell coordinate, mass density and temperature (electron and ion) respectively then with known values for $(r, \rho, T_{e,i})^{n-1}$ and $u^{n-1/2}$ $(r, \rho)^n$ we determine T^n, $u^{n+1/2}$, $(r, \rho)^{n+1}$. All basic quantities are thereby advanced one step in time. Due to the non-linearity of the $T_{e,i}$ in the energy equation, this equation is solved by iteration.

Since the temperature equations are solved implicitly, the solution for the temperature is stable for all time steps. However, the time step should be chosen carefully in order to obtain results within a desirable accuracy. The maximum value of Δt is restricted by the Courant-Friedrichs-Lewy conditions and is given as

$$\Delta t^{n+\frac{1}{2}} < \frac{a_1 Min(r_{j+1}^n - r_j^n)}{c_n}$$

The time step is also constrained by the maximum variation allowed in the hydrodynamic velocity and in the ion and electron temperatures.

5.1.11 LASER PROFILE:

In our simulations we use two types of laser beam time profiles. These are gaussian and trapezoid profiles. The maximum power attributed to a given beam ranges from 10^{16} Wm^{-2} to 10^{18} Wm^{-2}. A detailed description of laser characteristics is given wherever they are used in the simulations sections.

5.2 INTEGRATION OF DSA CODE IN MEDUSA:

The atomic physics tables developed by Lee[5/2] contain the emissivity and the microscopic cross-section area at a given temperature and ion density. These quantities are in MKS units, watts/ion and m^2, respectively. For the transfer equation we need the absorption coefficient and the initial intensity. In order to find the relation between given variables and required variables, consider the radiative transfer equation and the energy balance equation

$$\mu\frac{\partial I}{\partial x} + (\sigma+\tau)I = S = \sigma B$$

$$u_\sigma^{n+1} = \frac{\eta}{c\sigma_p^*}\left[\int_0^\infty \sigma^* I_0 d\nu + \frac{u_\sigma^n}{\Delta t\beta^*}\right]$$

$$\text{where} \qquad \beta = \frac{4aT^3}{c_v}$$

(5.2.01)

where I is the specific intensity in W m^{-2}, σ is the absorption coefficient in m^{-1}, S is the rate of energy emission due to spontaneous processes, c_v is the specific heat per unit volume and c is the speed of light in m/sec and B is the specific intensity.

A careful analysis shows that one can relate the emissivity and the microscopic cross-section area to the specific intensity and absorption coefficient as

$$B = \frac{N_i P\ \Delta x}{4\pi} \qquad \text{and} \qquad \sigma = N_i A_x$$

(5.2.02)

where P: is the rate of energy emitted W/ion

A_x: is the microscopic cross-sectional area in m^2

N_i: is the ion density per unit volume

The values of the emissivity and cross-section area are obtained through interpolation at a given temperature and density by calling subroutine DINTRP. If the temperature is less than 10 ev then the emissivity is taken to be Planckian, and

the cross-sectional area is obtained by calling the function named CIGMA. When CIGMA is called to obtain the absorption coefficient σ, then

$$\sigma = \frac{M \bar{A}_x}{N_A}$$

(5.2.03)

where A'_x is obtained from CIGMA, N_A is the Avogadro number, and M is the atomic mass. The specific heat is obtained from the EOS subroutine, and is given as

$$c_v = \rho_3 \frac{[c_{vi} + c_{ve}]}{10.0}$$

(5.2.04)

Where ρ_3 corresponds to mass density at time step 3 and c_{vi} and c_{ve} are the specific heats obtained from EOS at time level 3.

The emitted power is defined as the power loss per unit mass from the plasma; therefore, it is proportional to the difference in the intensity at the adjacent cell boundaries obtained after solving the transfer equation at time level 3. This can be expressed as

$$BREMS_i = \frac{2\pi}{\Delta m_i} \Sigma_g A_{xg} [\Sigma_m (I_{mgi+\frac{1}{2}} - I_{mgi-\frac{1}{2}}) \omega_m]$$

(5.2.05)

The present radiation code is invoked by setting SAHA=3.1. In all of the simulations the foil is taken to be **aluminium** and the **flux limiter** is taken to be 0.25. Variables such as temperature, pressure, velocity, average Z and mass density as a function of space are stored into file named "**out**". Quantities such as the ablation pressure, ablated mass, average Z, thermal and kinetic energy and emission to the left and right end of the plasma, as a function of time are stored into "**abl.out**". The **ablated mass** is defined as the mass contained between the outside cell and the last cell in the plasma in which an outward velocity is obtained. The **ablation pressure**

is defined as the pressure of the cell embodied in the ablative surface. The option of a trapezoid time profile for the laser beam has been added. This can be invoked by setting GAUSS =-2.0, PLENTH="rise time (assumed to be same as fall time)". The input file for MEDUSA is "**mds.in**" and it is given below, this will allow another user to reproduce the results presented here without any uncertainty in the initial conditions that are used. Important variables are bolded.

```
F0000000  0  1
 ENERGY : 1.00 JOULES    FOCAL SPOT DIA: 70 MICRONS
 TARGET : ALUMINUM       2.0 NS PULSE

 ==========================================================
 &NEWRUN
  AK0=0.10,                AK1=0.10,                AK2=0.10,
  AK3=0.10,                AK4=0.10,                AK5=0.00,
  ANABS=1.0,               ANPULS=1.0,
  BNEUM=2.0,
  DTEMAX=0.1,              DTIMAX=0.1,              DUMAX=0.1,
  DTPRNT=2.5D-10,          DELTAT=1.0D-12,          DRGLAS=0.0,
  DRPLAS=0.0,              DEUTER=0.0
  FHOT=0.0,                FTHOT=0.0,               FLIMIT=1.00,
  FNE=1.0,
  GAUSS= -2.0,             GAMMAE=1.66666667,       GAMMAI=1.66666667,
  HELIU3=0.0,              HELIU4=0.0,              HYDROG=0.0,
  LAMDA1=2.48D-06,
  MESH=40,                 MXDUMP=10,
  NITMAX=50,               NCASE=1,                 NRUN=99999,
  NLABS=.TRUE.,            NLMOVE=.TRIE.,           NLBURN=.FALSE.,
  NLCRI1=.TRUE.,           NLBRMS=.TRUE.,           NLITE=.TRUE.,
  NLDEPO=.FALSE.,          NLDUMP=.FALSE.,          NLFUSE=.FALSE.,
  NREP=0,                  NTRLMS=0.0,              NSLEDG=9999,
  NDUMP=10,                NETRAL=0.0,              NFILM=1,
  NGROUP=5,                NHDCPY=100,              NIN=5,
  NLCHED=.FALSE.,          NLEDGE=10,               NLEMP=.TRUE.,
  NLFILM=.TRUE.,           NLHCPY=.FALSE.,          NLPRNT=.TRUE.,
  NLREPT=.FALSE.,          NONLIN=1,                NSHELL=150,
  NP1=1,                   NP2=40,                  NP3=1,
  NPRNT = 50000,           NGEOM=1,                 NREP=0,
  NLECON=.TRUE.,           NLICON=.TRUE.,           NLOMT2(11)=.TRUE.,
  NLPFE=.FALSE.,           NLPFI=.TRUE.,            NLX=.TRUE.,
  NLOMT2(6)=.TRUE.,        NLOMT2(7)=.TRUE.,
  OUTAMI=1.0,
  PIQ(55)=2.0,             PONDF=-1.0,              PLENTH=1.0D-10,
  PMULT=2.0,               PMAX=3.16D+17,
  QSHELL(1)=0.97,
  RINI=1.0D-04,            ROGLAS=0.0,              ROPLAS=0.0,
  RHOGAS=2700.0,           RHOINI=2700.0,           RSHELL=1.0D-04,
  RHOT=0.0,
  SAHA=3.1,                STATE=-1.0,              SIMULT=1.0,
  SCR=1.0,                 SCRHO=1.0,               SCTE=1.0,
  SCTI=1.0,                SCTIME=1.0,              SCP=1.0,
  TEINI=3.0D02,            TIINI=3.0D02,            TINUCL=1.0D+07,
  TRITIU=0.0,              TON=0.0,                 TOFF=3.9D-09,
  TSTOP=5.0D-09,
  XMASS=26.9815,           XTRA=1.0,                XZ=13.0,
  ZGLAS=0.0,               ZPLAS=0.0,
 &END
  HNUMIN=8000.0,           HNUMAX=9000.0,           NLEMRA=.FALSE.
```

5.3 MEDUSA SIMULATIONS:

This section includes the MEDUSA simulations. The main objective is to validate Marchand's Model with the present code. This is done by comparing the MEDUSA simulations which use Marchand's model and the present code. It will be shown that there are cases where the two algorithms yield different results. These results will be presented followed by a discussion of which algorithm appears to be more accurate. Since Marchand's model was successfully tested against experimental observation, we believe that the present code must also confirm the same experimental observations.

The graphs to be presented in this section reflect the consistency and the differences of the two models. It is observed that Marchand's model works well for a trapezoid profile beam, but appears to give erroneous results when a gaussian profile beam is used. The effects of radiation transport are the subject of this section. The input file for MEDUSA is given on the previous page.

Figure 5.1 a, b, c

This graph represents the electron temperature and normalized mass density of the plasma as a function of space using the DSA model and Marchand's 2-cell simplified model. The laser beam has a trapezoid temporal profile (with RISE TIME = 1.0E-10 sec, TOFF = 4.0E-09 sec and PMAX = 3.16E17 Wm^{-2}, λ = 2.48E-07). These graphs correspond to different time steps and are presented here to show the consistency between the present model and Marchand's model at various time steps.

Figure 5.2 a, b, c

This graph represents the pressure and normalized mass density of the plasma as a function of space with the DSA model and Marchand's model. The laser beam is the same as the one used in Fig. 5.1 (trapezoid). Each graph can be viewed as a snap shot of the pressure and the mass density at different times. Again the consistency between the two models is evident.

Figure 5.3

This graph represents the ablation mass as a function of time with the DSA model and Marchand's model. The laser profile is the same as in Fig. 5.1.

Figure 5.4

This graph represents the ablation pressure as a function of time with the DSA model and Marchand's model. The laser profile is the same as Fig. 5.1.

Figure 5.5 a,b,c

These graphs represent the electron temperature and mass density as a function of space, when a gaussian laser profile (with FWHM = 1.7E-09 sec, PMAX = 5.0E16 Wm^{-2}, λ = 0.35E-06) is used. This figure shows that when a gaussian profile is used the two models do not give as consistent electron temperature as they did for trapezoid laser profile.

Figure 5.6 a,b,c

Here the pressure and mass density are shown as a function of space, when a gaussian profile for the laser beam is used (same as in Fig. 5.5). Even though the electron temperature was the same for both models, the pressure is not the same. The inconsistency in pressure is quiet conspicuous, the dip in pressure about the ablation surface in Fig. 5.6 b of Marchand's model appears to be nonphysical.

Figure 5.7

This graph represents the ablation mass of the plasma when a laser beam with a gaussian profile is used. Here the inconsistency is so conspicuous that one needs to reject either the DSA model or Marchand's model. It appears that the DSA model is more accurate than Marchand's model, because in Figure 5.3 the intensity is higher than in Fig. 5.7, which implies that the ablation mass in Fig. 5.7 should be less than the ablation mass in Fig. 5.3. This is not true in Marchand's model.

Figure 5.8

This graph represents the ablation pressure of the plasma when a laser beam with a gaussian profile is used. Even though the ablation mass from the two models is quiet different, the ablation pressure is not very different. This reflects the complexity of the radiation transport, that is, consistency in one result does not necessary imply that other parameters are consistent too.

Figure 5.9 a,b,c,d,e

These graphs show the effects of radiation transport on the ablated mass, ablation pressure, kinetic energy, thermal energy and ion energy. The laser profile is a trapezoid (with PLENTH = 1.0E-10, PMAX = 3.16E17). In these graphs results of MEDUSA with radiation transport (by invoking DSA model or Marchand model) and with no radiation transport (it implies that all radiation emitted is lost rather than being transported) are presented.

Fig. 5.9 a,b show the effect of radiation transport on the ablation mass and ablation pressure. Mora[5/34] has shown that the ablation mass and ablation pressure are proportional to intensity and to the critical density of the plasma and are given as

$$m_{abl} \propto I_o^{\frac{1}{2}} n_c^{\frac{1}{4}} \qquad P_{abl} \propto I_o^{\frac{3}{4}} n_c^{\frac{1}{8}}$$

These relations indicate that ablation pressure is less sensitive to radiation transport compared to ablation mass. The weak dependence of pressure on radiation is due to the fact that with radiation transport the thermal energy is converted into x-rays which can escape the plasma, this conversion reduces the ablation pressure. Radiation transport on the other hand transports energy to higher density plasma which in turn contributes to an increase in ablation pressure. The graphs in Fig. 5.9 a,b qualitatively confirm such relations.

When radiation transport is not included, all of the energy emitted due to bremsstrahlung is taken to be a loss. With radiation transport some of the energy

is transported to a colder dense plasma. Therefore, it is expected that when radiation transport is included the kinetic energy, ion energy and thermal energy should be relatively large compared to the case when no radiation is included. This conclusion is qualitatively confirmed from Fig. 5.9 c,d,e.

Figure 5.1 a

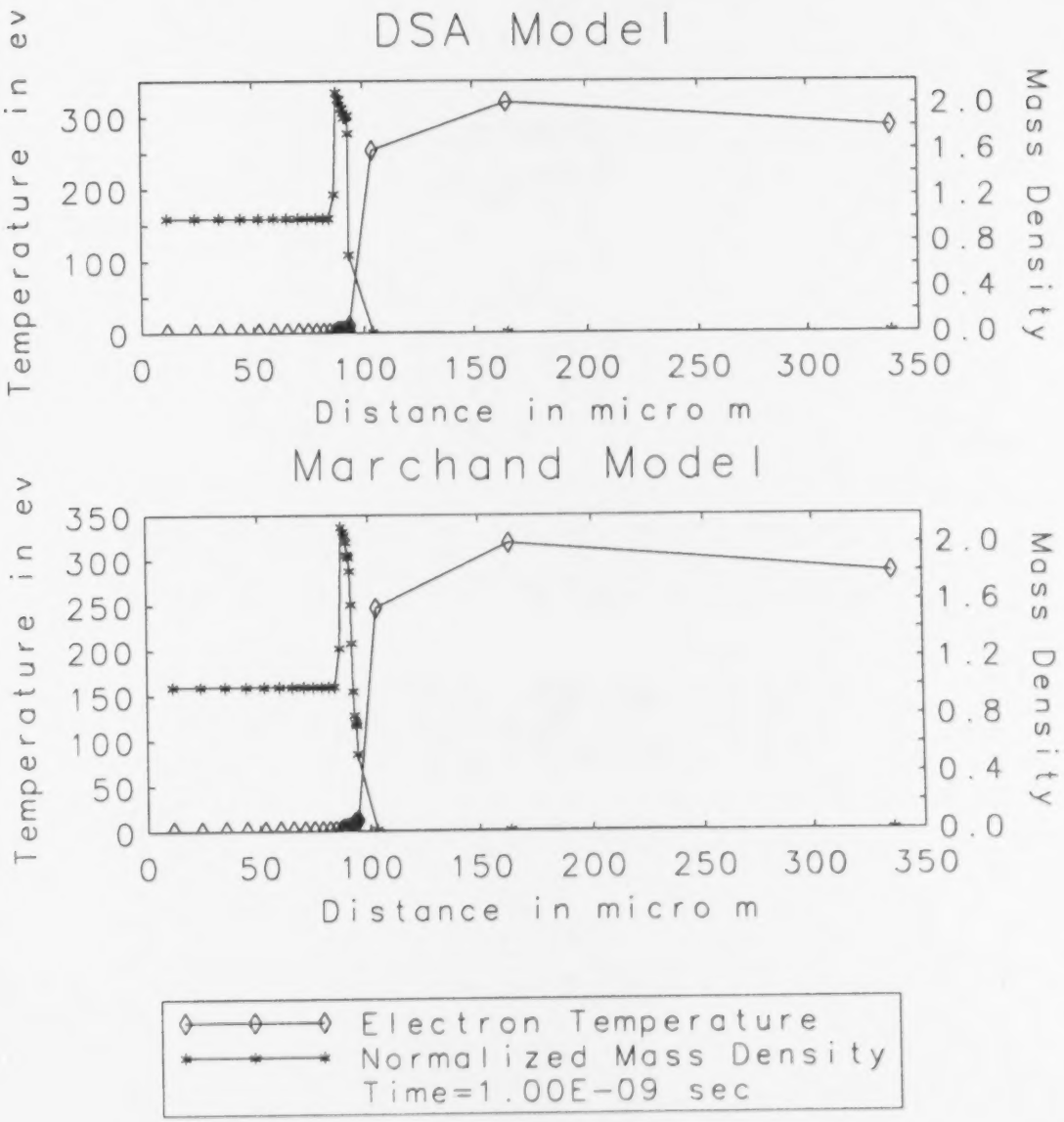

DSA Model
Temperature in ev
Mass Density
Distance in micro m
Marchand Model
Temperature in ev
Mass Density
Distance in micro m
Electron Temperature
Normalized Mass Density
Time=1.00E-09 sec

Figure 5.1 b

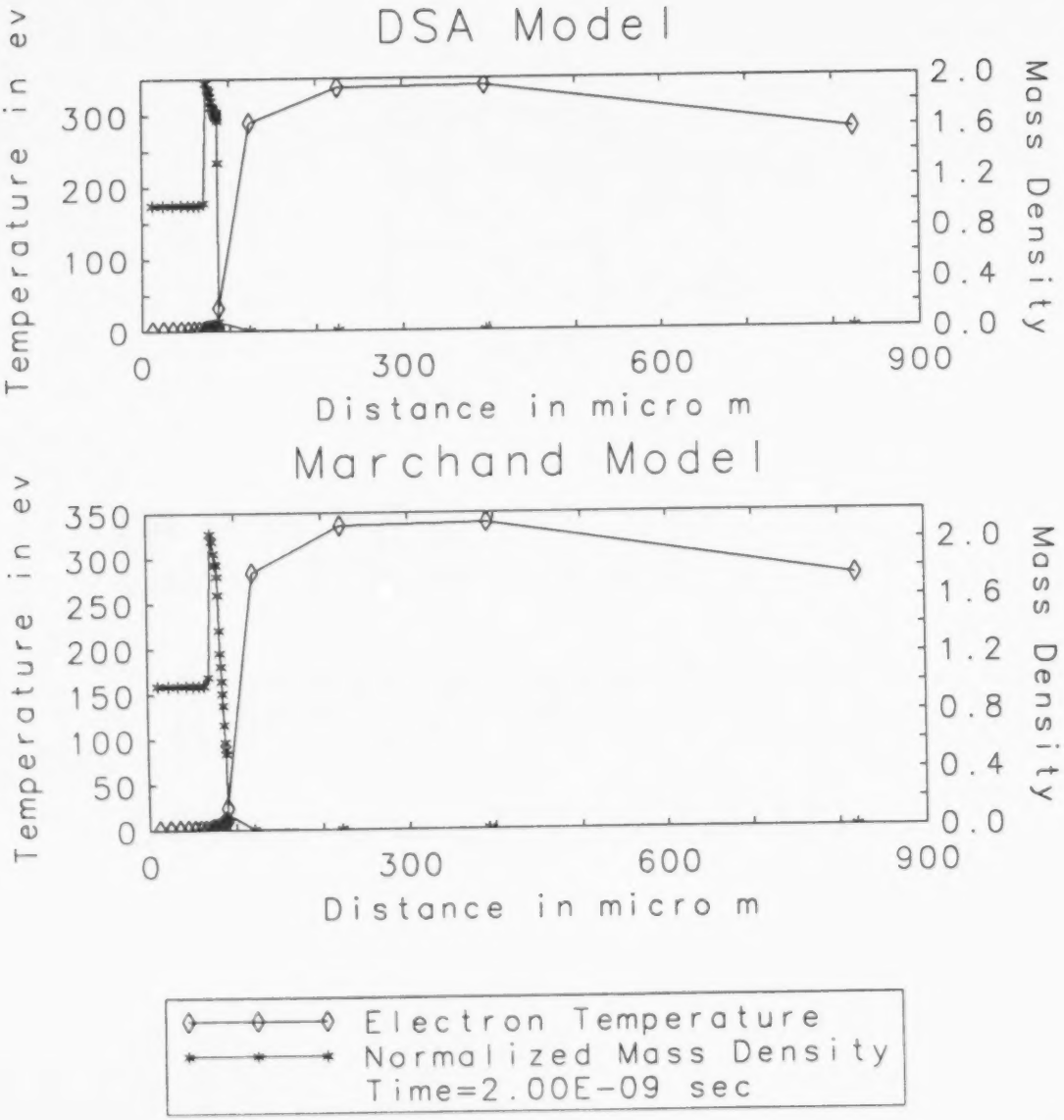

DSA Model
Temperature in ev
Mass Density
300
200
100
0
2.0
1.6
1.2
0.8
0.4
0.0
0
300
600
900
Distance in micro m
Marchand Model
Temperature in ev
Mass Density
350
300
250
200
150
100
50
0
2.0
1.6
1.2
0.8
0.4
0.0
0
300
600
900
Distance in micro m
Electron Temperature
Normalized Mass Density
Time=2.00E-09 sec

Figure 5.1 c

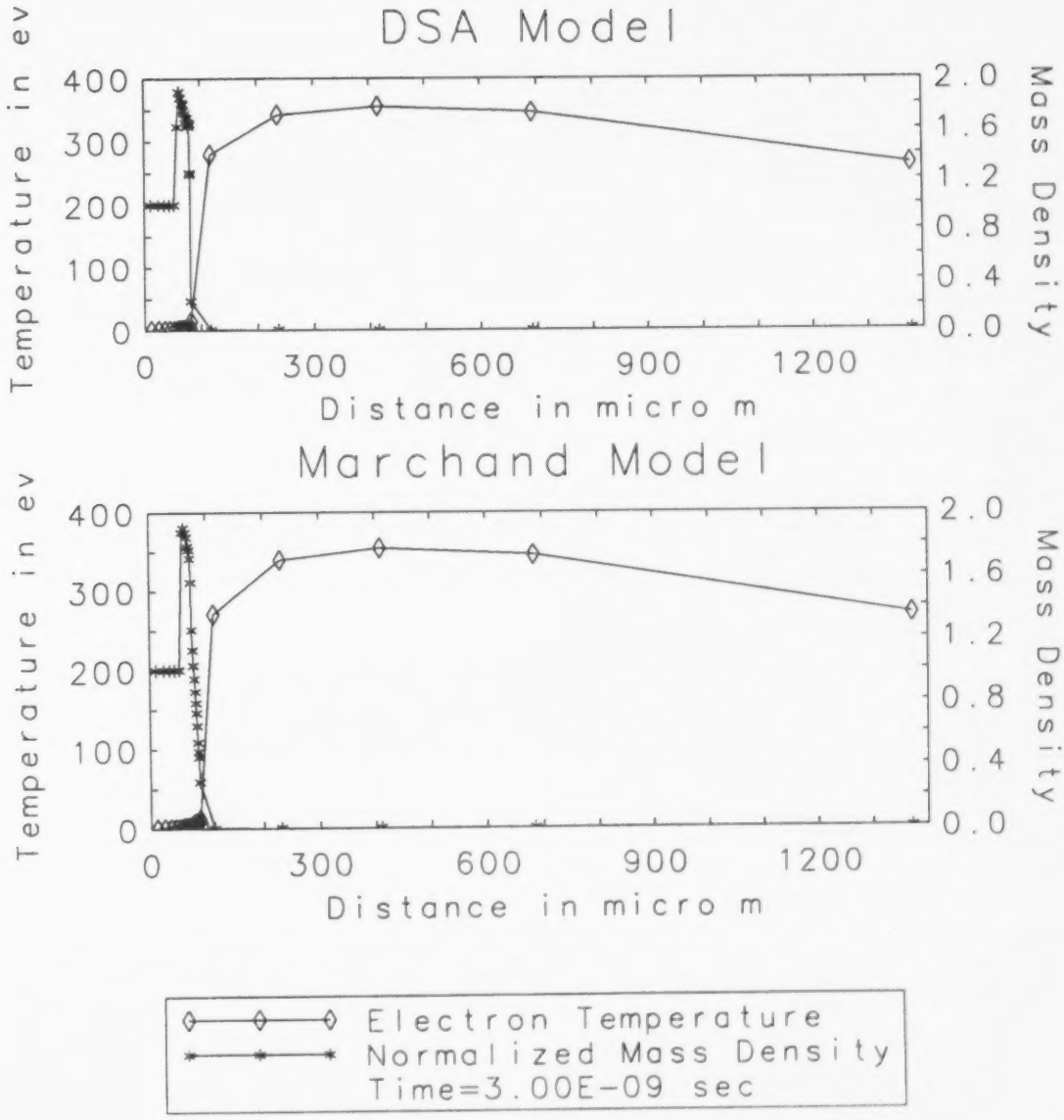

DSA Model
Temperature in ev
Mass Density
400
300
200
100
0
2.0
1.6
1.2
0.8
0.4
0.0
0
300
600
900
1200
Distance in micro m
Marchand Model
Temperature in ev
Mass Density
400
300
200
100
0
2.0
1.6
1.2
0.8
0.4
0.0
0
300
600
900
1200
Distance in micro m
Electron Temperature
Normalized Mass Density
Time=3.00E-09 sec

Figure 5.2 a

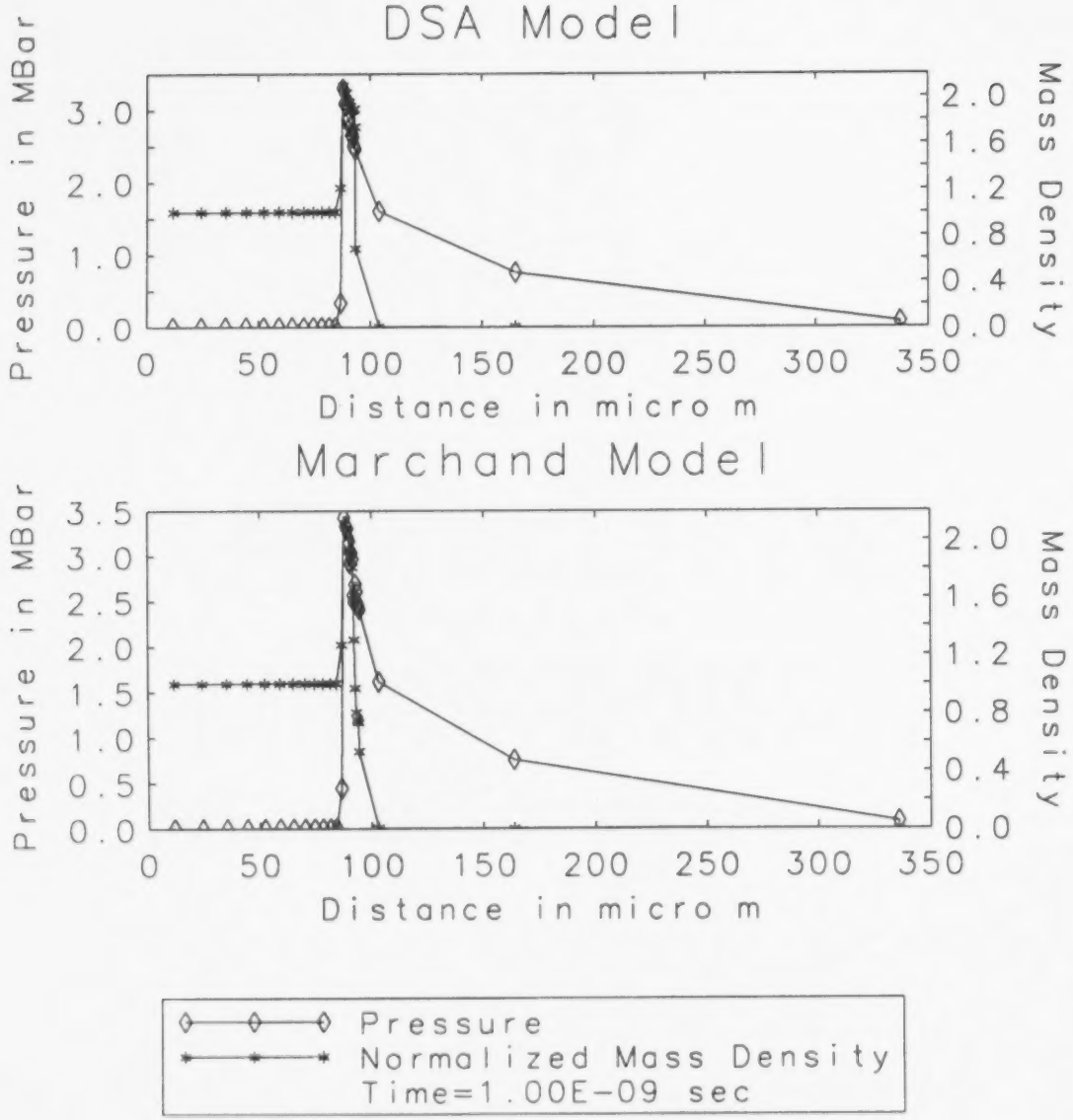

DSA Model
Pressure in MBar
Mass Density
3.0
2.0
1.0
0.0
2.0
1.6
1.2
0.8
0.4
0.0
0
50
100
150
200
250
300
350
Distance in micro m
Marchand Model
Pressure in MBar
Mass Density
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
2.0
1.6
1.2
0.8
0.4
0.0
0
50
100
150
200
250
300
350
Distance in micro m
Pressure
Normalized Mass Density
Time=1.00E-09 sec

Figure 5.2 b

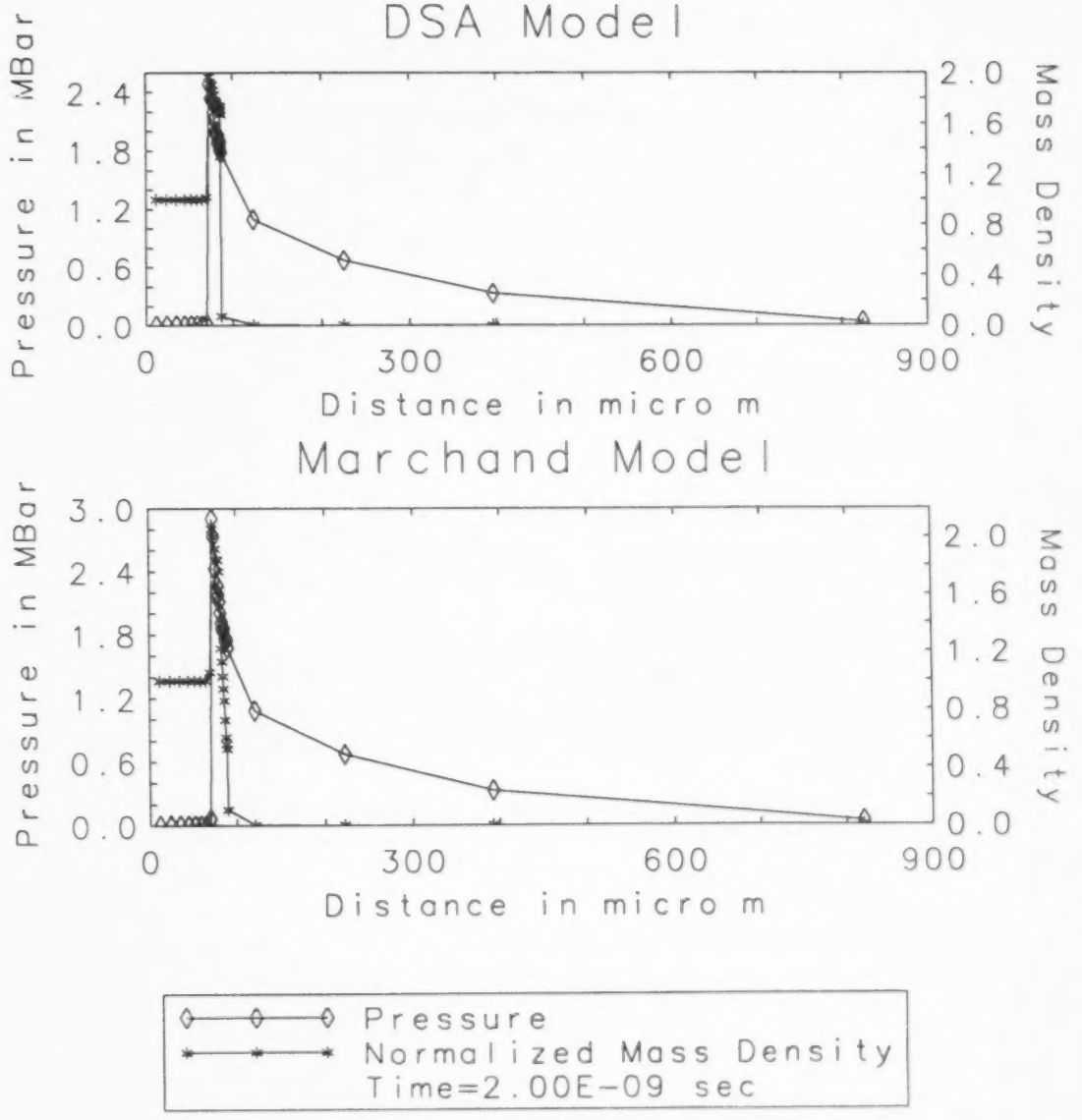

DSA Model
Pressure in MBar
Mass Density
2.4
1.8
1.2
0.6
0.0
2.0
1.6
1.2
0.8
0.4
0.0
0
300
600
900
Distance in micro m
Marchand Model
Pressure in MBar
Mass Density
3.0
2.4
1.8
1.2
0.6
0.0
2.0
1.6
1.2
0.8
0.4
0.0
0
300
600
900
Distance in micro m
Pressure
Normalized Mass Density
Time=2.00E-09 sec

Figure 5.2 c

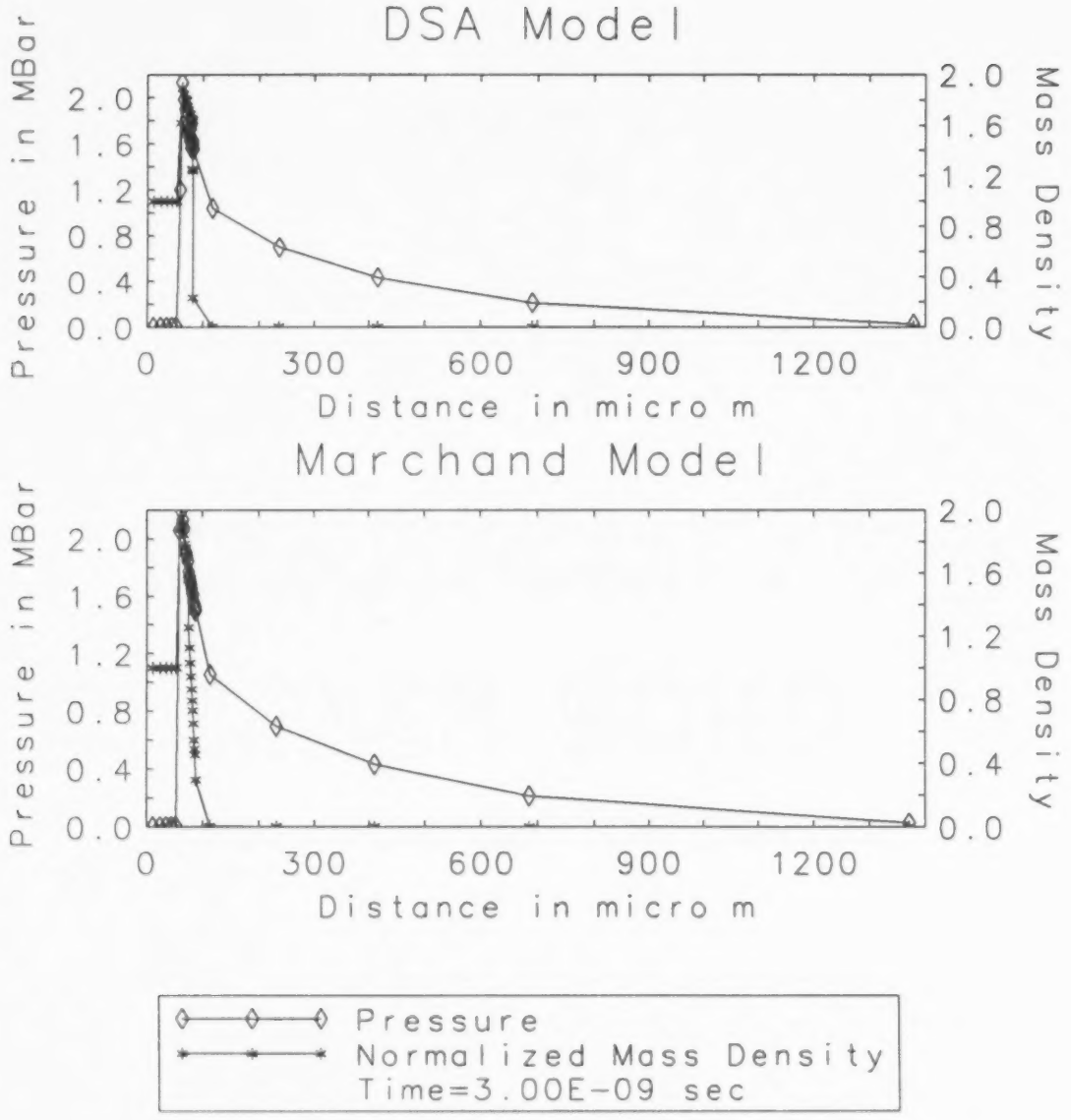

DSA Model
Pressure in MBar
Mass Density
2.0
1.6
1.2
0.8
0.4
0.0
0
300
600
900
1200
Distance in micro m
Marchand Model
Pressure in MBar
Mass Density
2.0
1.6
1.2
0.8
0.4
0.0
0
300
600
900
1200
Distance in micro m
Pressure
Normalized Mass Density
Time=3.00E-09 sec

Figure 5.3

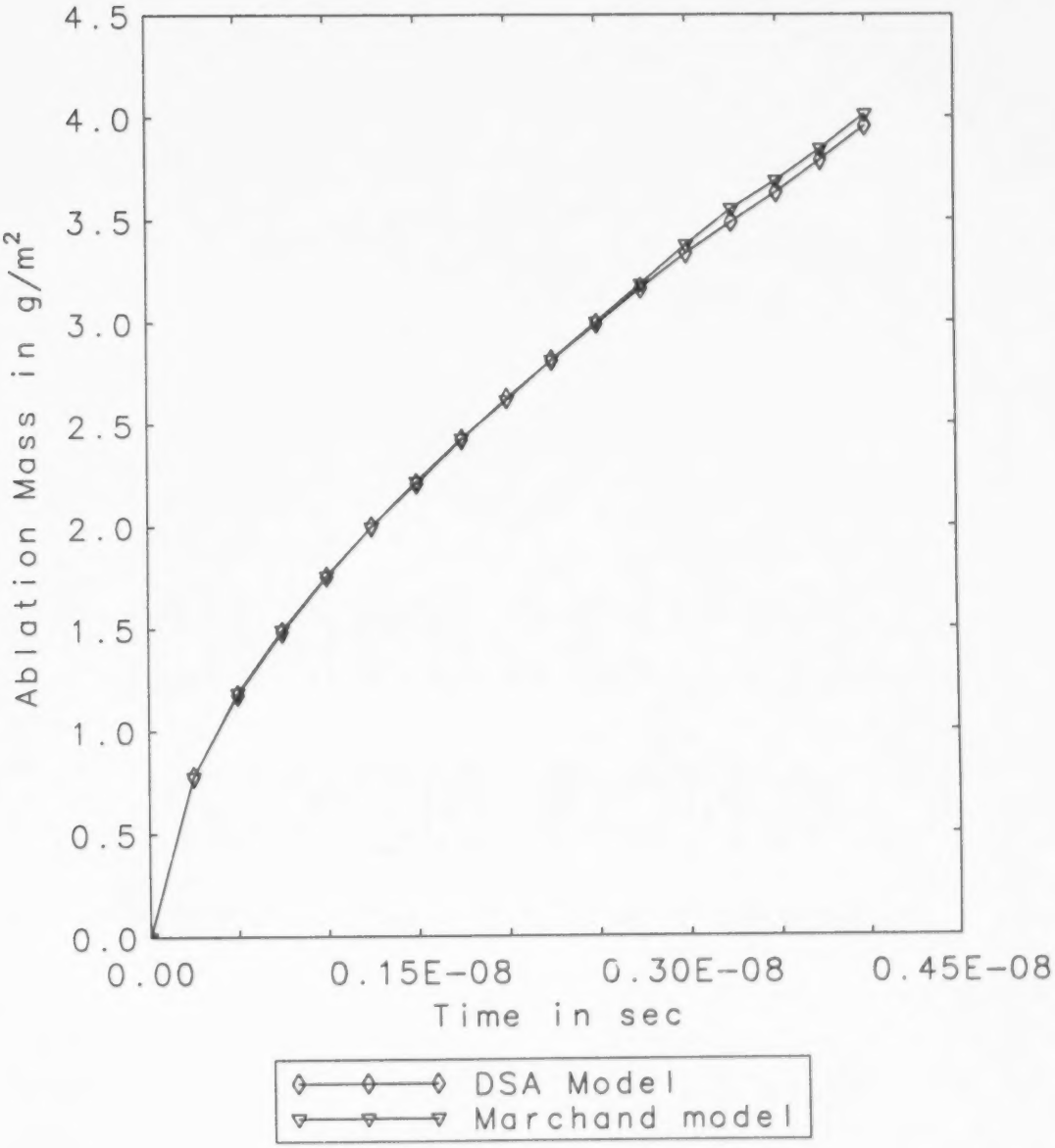

4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Ablation Mass in g/m2
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec
DSA Model
Marchand model

Figure 5.4

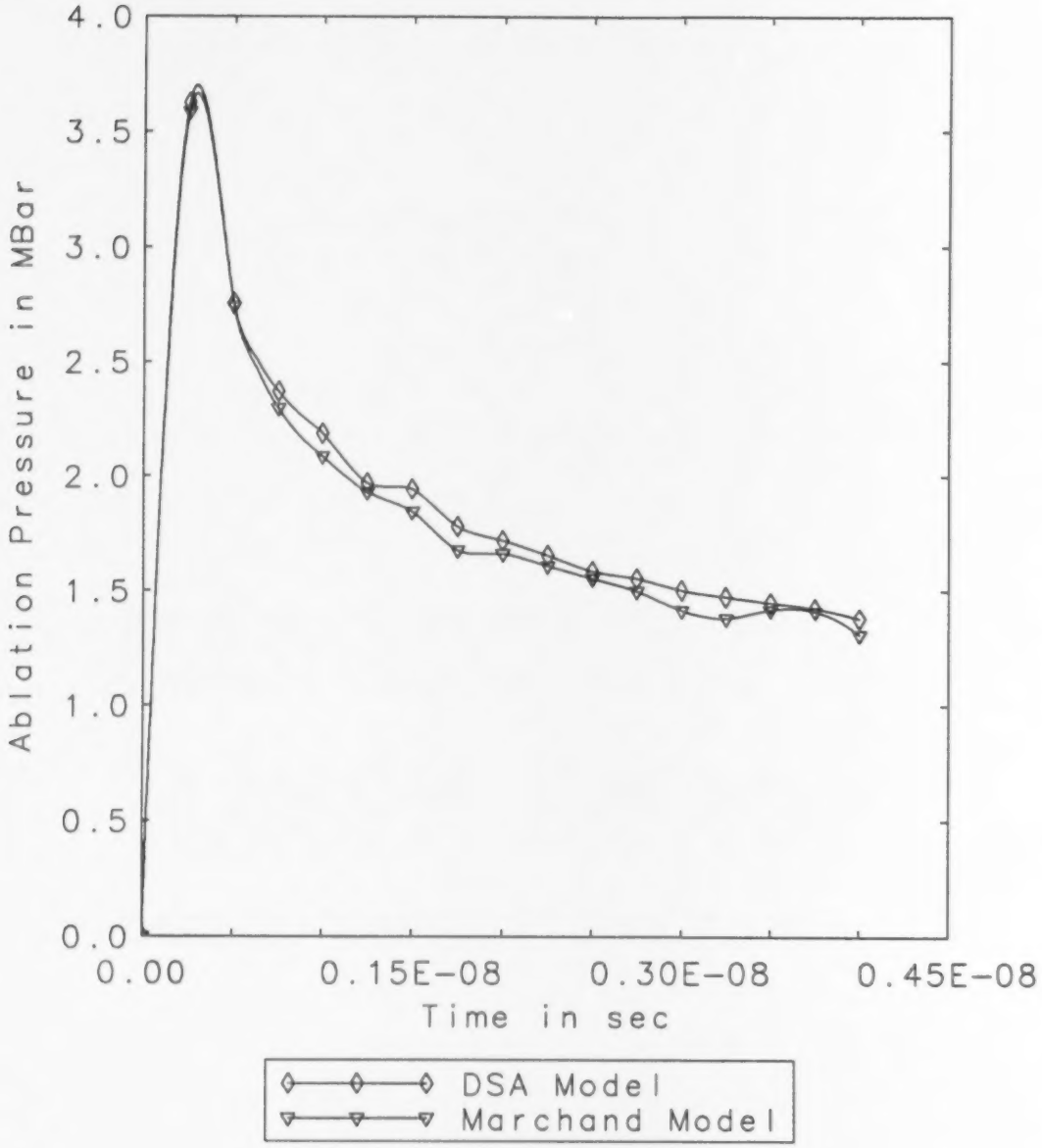

4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Ablation Pressure in MBar
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec
DSA Model
Marchand Model

Figure 5.5 a

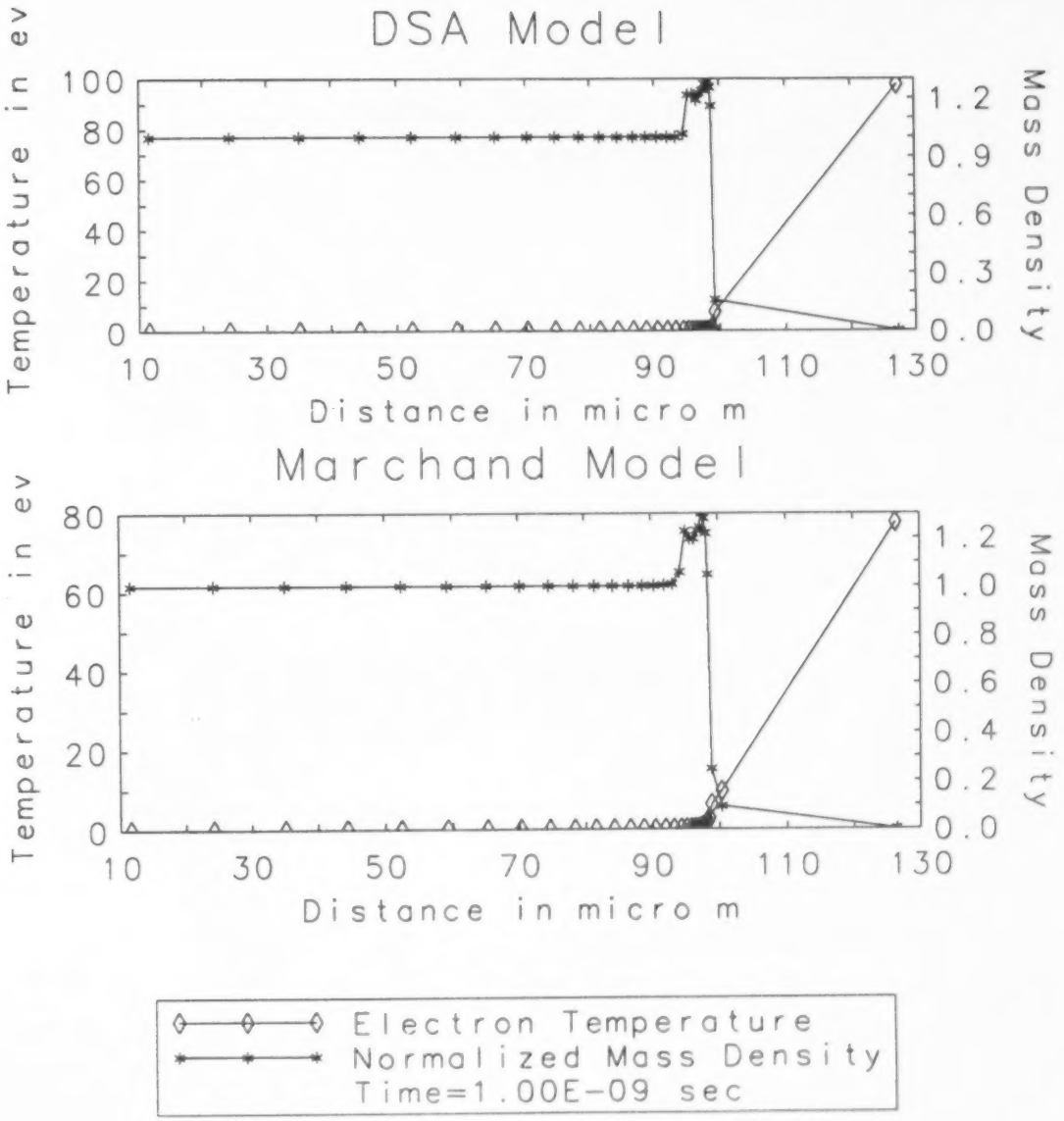

DSA Model
Temperature in ev
Mass Density
Distance in micro m
Marchand Model
Temperature in ev
Mass Density
Distance in micro m
Electron Temperature
Normalized Mass Density
Time=1.00E-09 sec

Figure 5.5 b

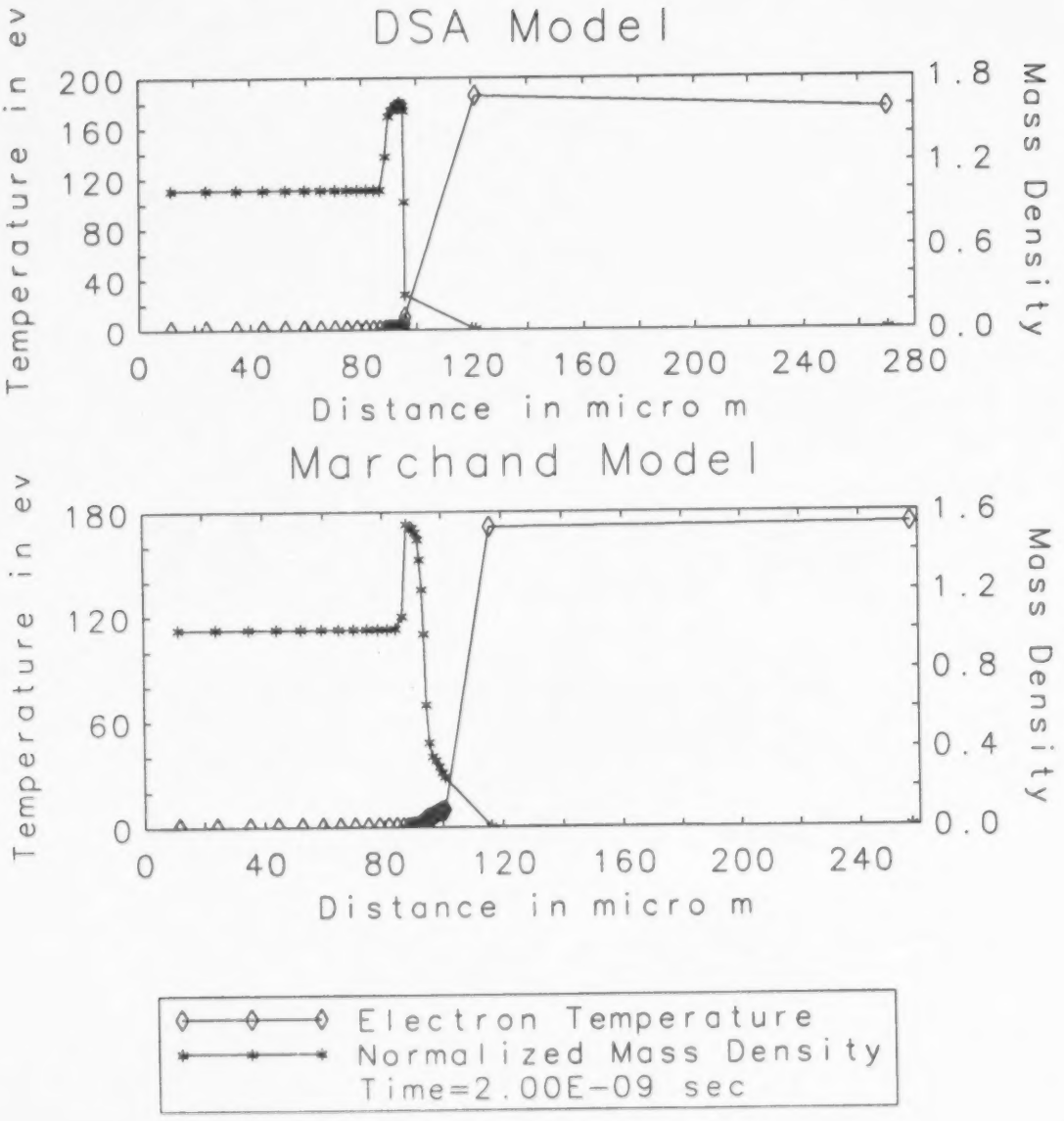

DSA Model
Temperature in ev
200
160
120
80
40
0
1.8
1.2
0.6
0.0
Mass Density
0
40
80
120
160
200
240
280
Distance in micro m
Marchand Model
Temperature in ev
180
120
60
0
1.6
1.2
0.8
0.4
0.0
Mass Density
0
40
80
120
160
200
240
Distance in micro m
Electron Temperature
Normalized Mass Density
Time=2.00E-09 sec

Figure 5.5 c

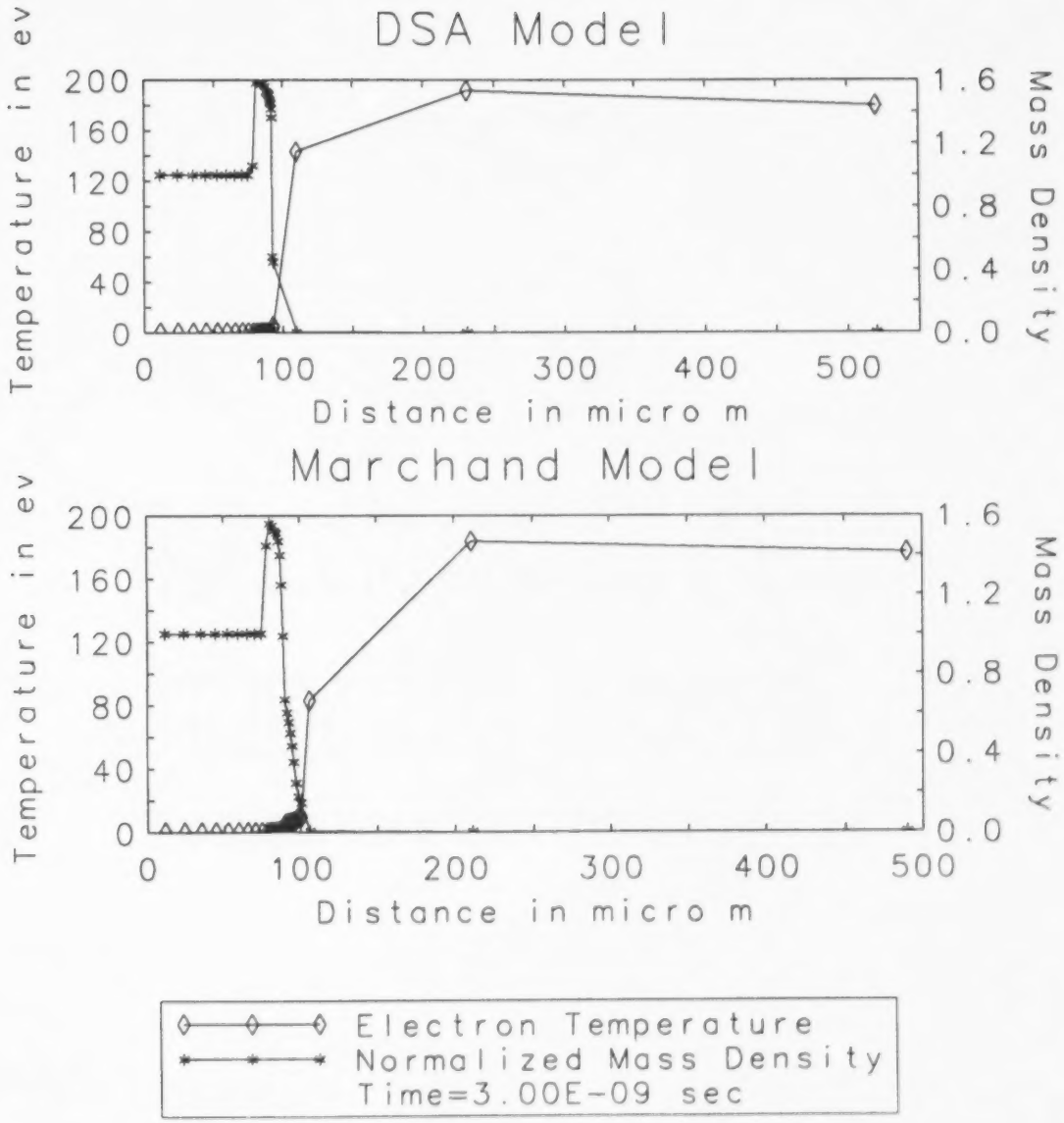

DSA Model
Temperature in ev
200
160
120
80
40
0
0
100
200
300
400
500
Distance in micro m
1.6
1.2
0.8
0.4
0.0
Mass Density
Marchand Model
Temperature in ev
200
160
120
80
40
0
0
100
200
300
400
500
Distance in micro m
1.6
1.2
0.8
0.4
0.0
Mass Density
Electron Temperature
Normalized Mass Density
Time=3.00E-09 sec

Figure 5.6 a

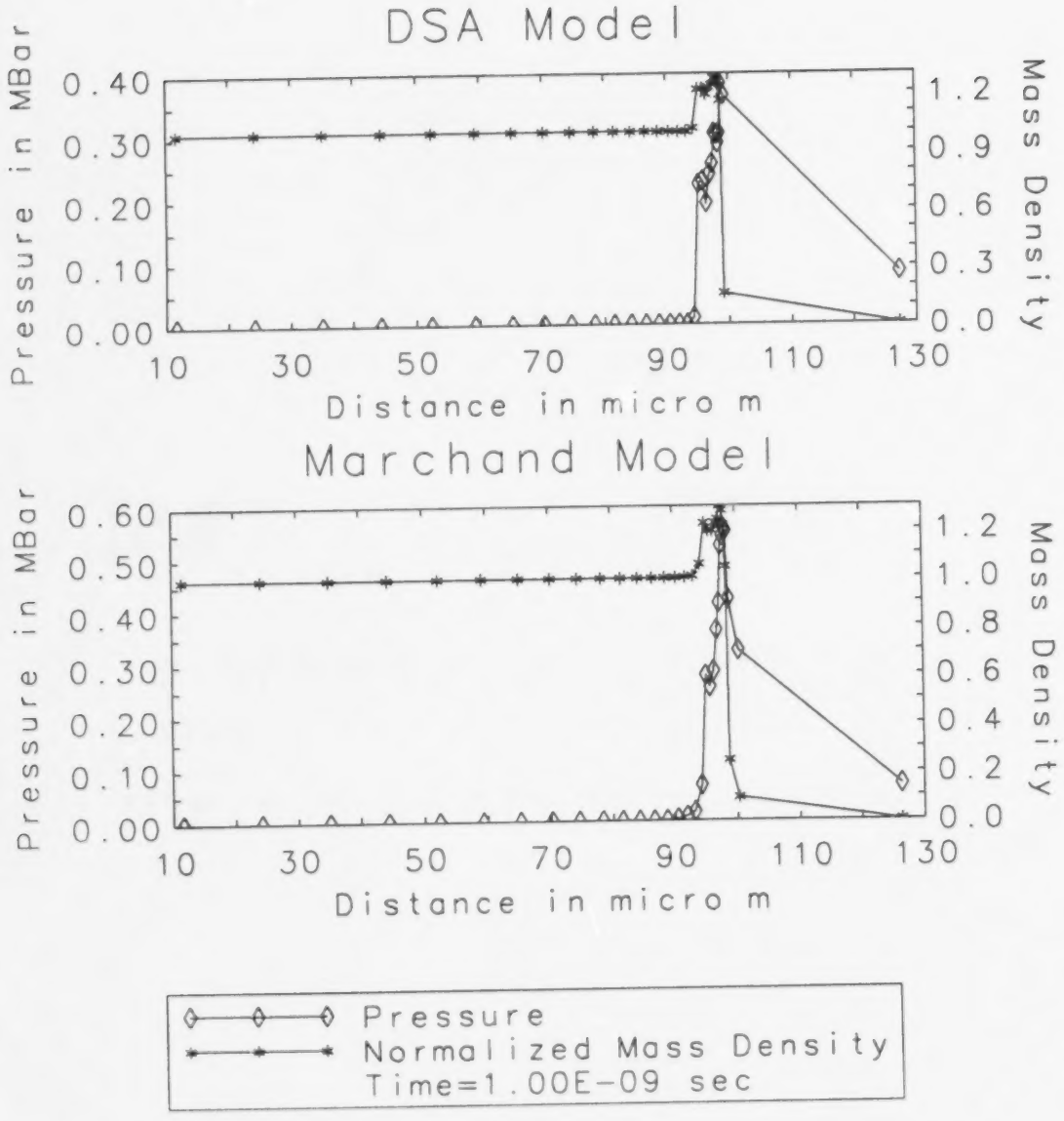

DSA Model
Pressure in MBar
0.40
0.30
0.20
0.10
0.00
1.2
0.9
0.6
0.3
0.0
Mass Density
10
30
50
70
90
110
130
Distance in micro m
Marchand Model
Pressure in MBar
0.60
0.50
0.40
0.30
0.20
0.10
0.00
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Mass Density
10
30
50
70
90
110
130
Distance in micro m
Pressure
Normalized Mass Density
Time=1.00E-09 sec

Figure 5.6 b

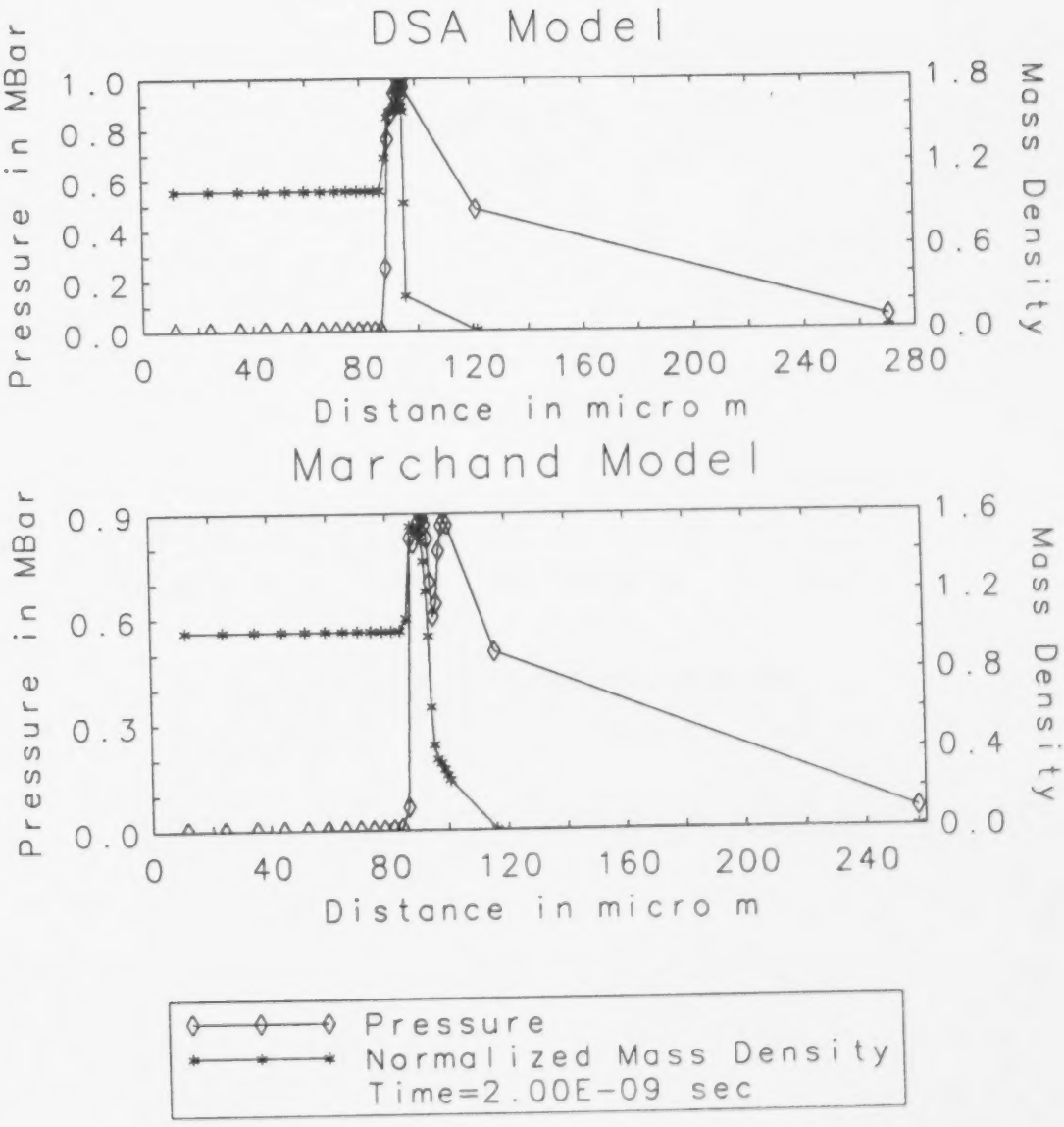

DSA Model
Pressure in MBar
1.0
0.8
0.6
0.4
0.2
0.0
1.8
1.2
0.6
0.0
Mass Density
0
40
80
120
160
200
240
280
Distance in micro m
Marchand Model
Pressure in MBar
0.9
0.6
0.3
0.0
1.6
1.2
0.8
0.4
0.0
Mass Density
0
40
80
120
160
200
240
Distance in micro m
Pressure
Normalized Mass Density
Time=2.00E-09 sec

Figure 5.6 c

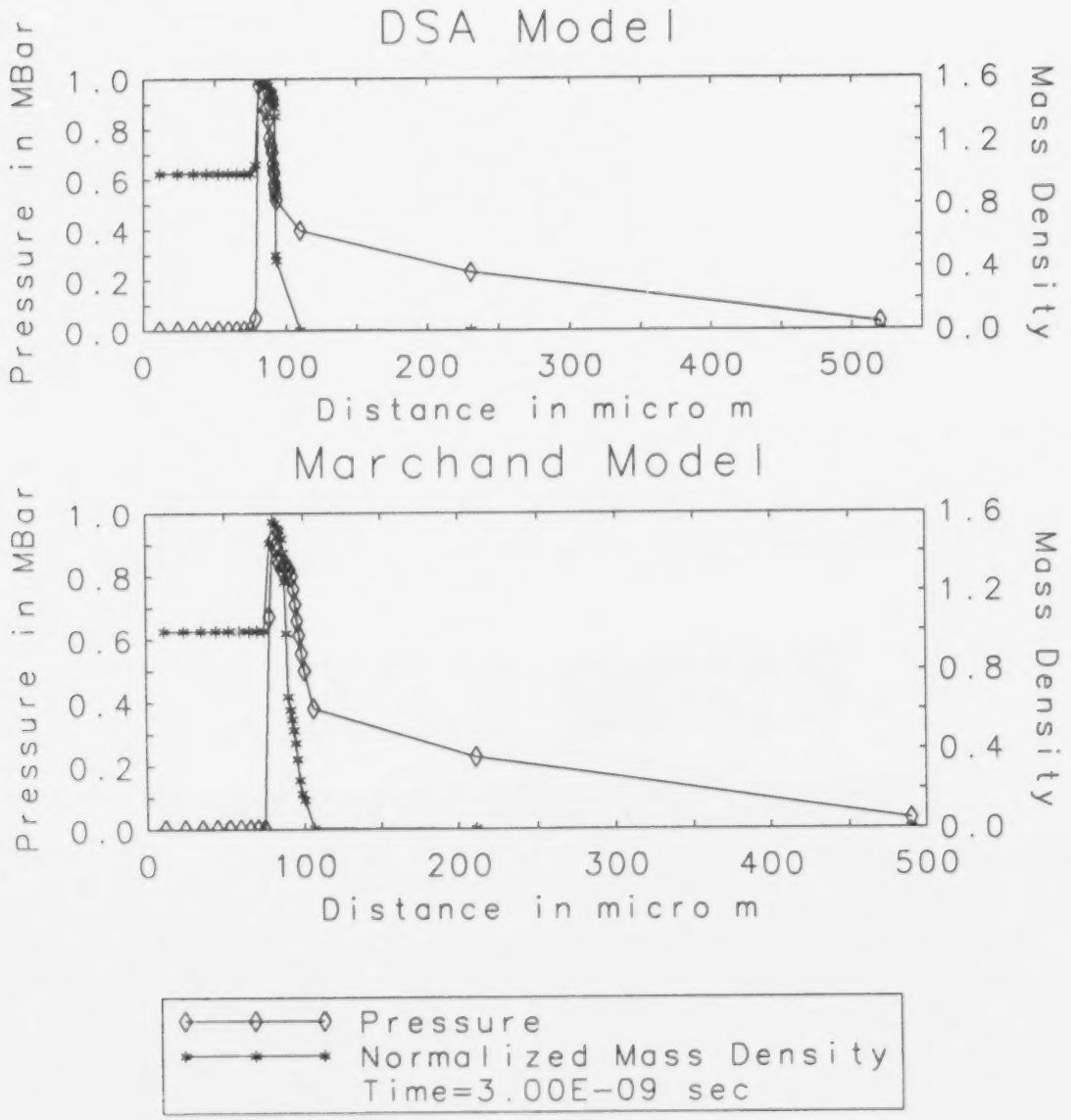

DSA Model
Pressure in MBar
Mass Density
1.0
0.8
0.6
0.4
0.2
0.0
1.6
1.2
0.8
0.4
0.0
0
100
200
300
400
500
Distance in micro m
Marchand Model
Pressure in MBar
Mass Density
Distance in micro m
Pressure
Normalized Mass Density
Time=3.00E-09 sec

Figure 5.7

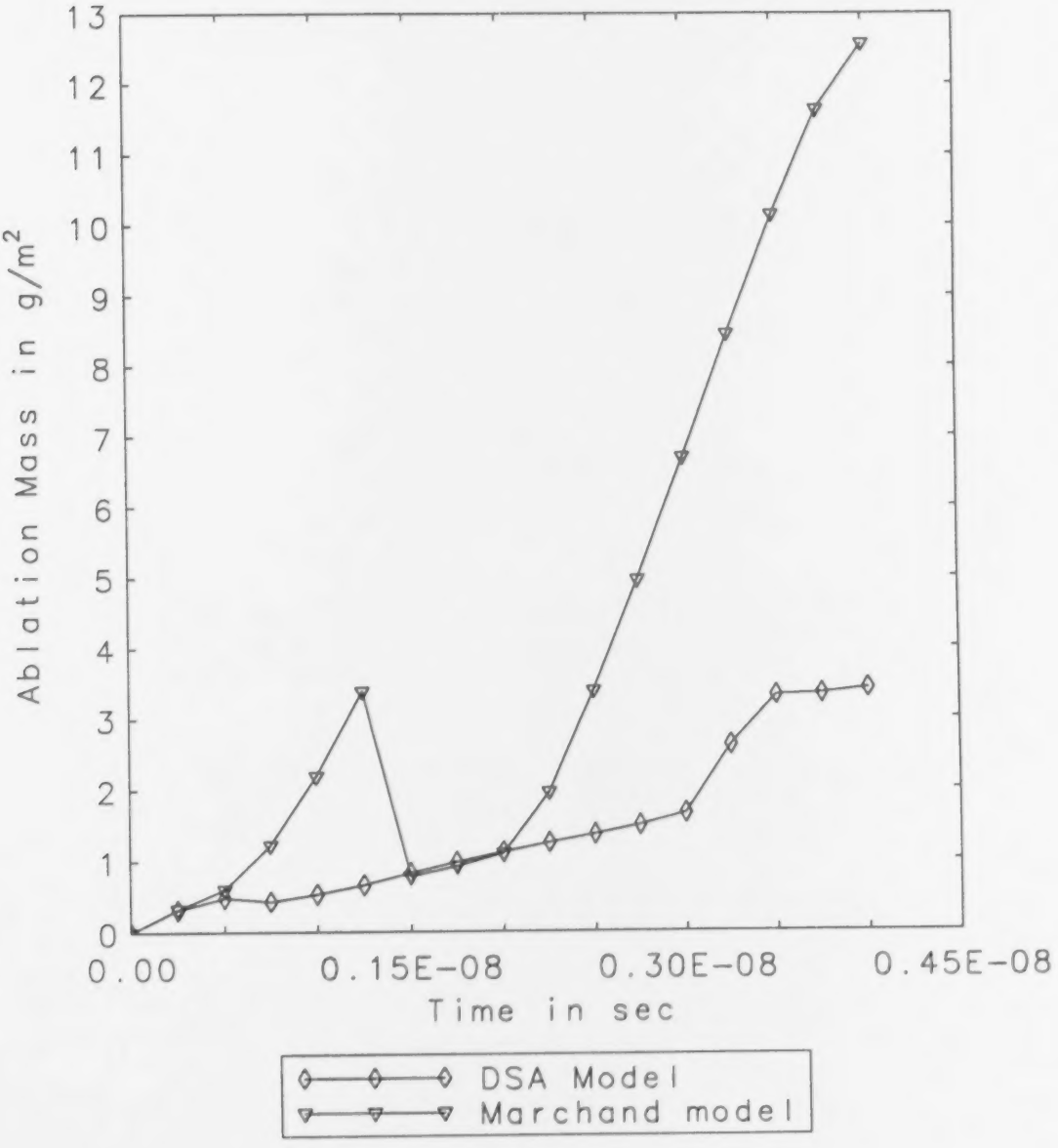

Ablation Mass in g/m2
13
12
11
10
9
8
7
6
5
4
3
2
1
0
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec
DSA Model
Marchand model

Figure 5.8

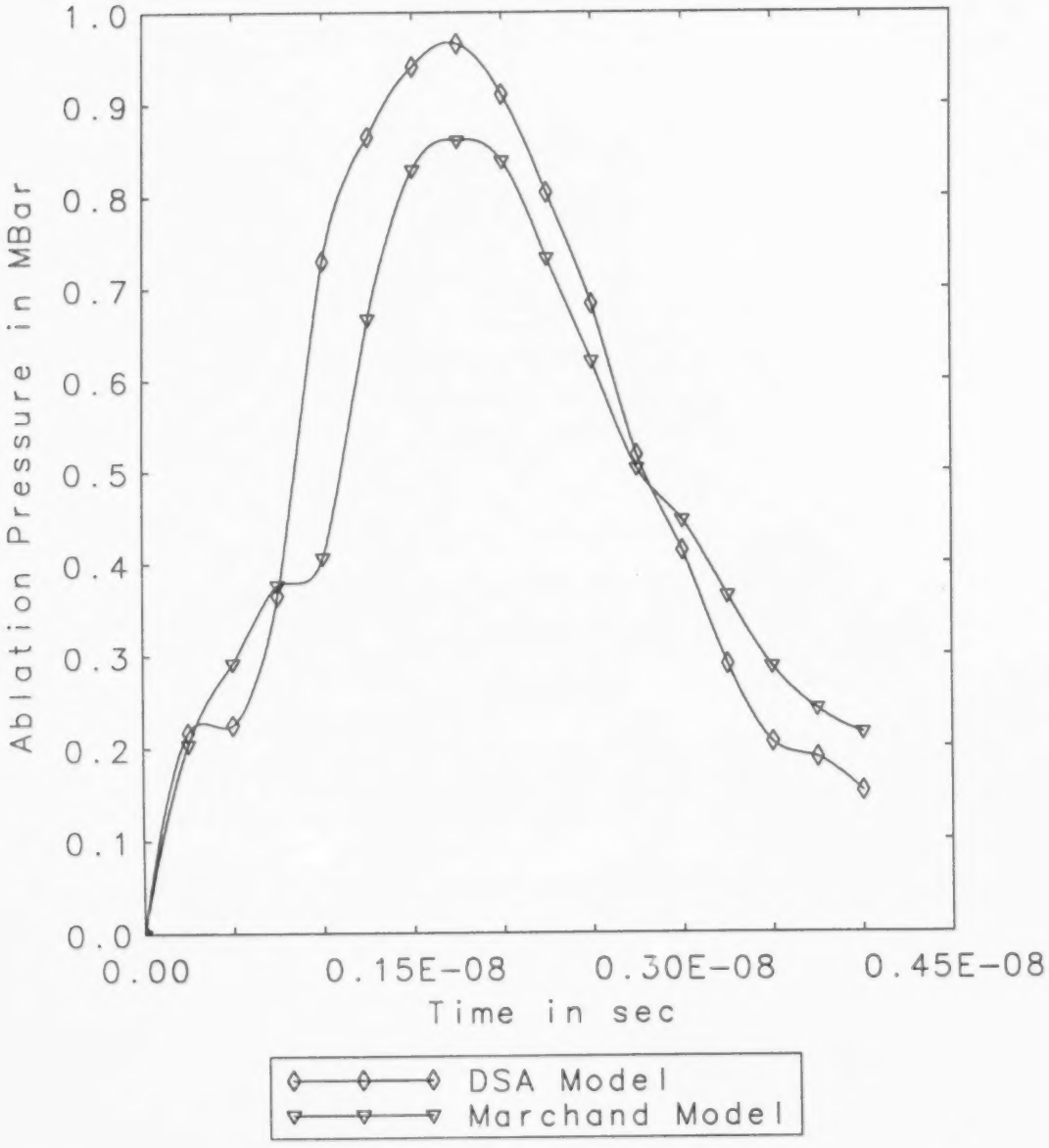

1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Ablation Pressure in MBar
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec
DSA Model
Marchand Model

Figure 5.9 a

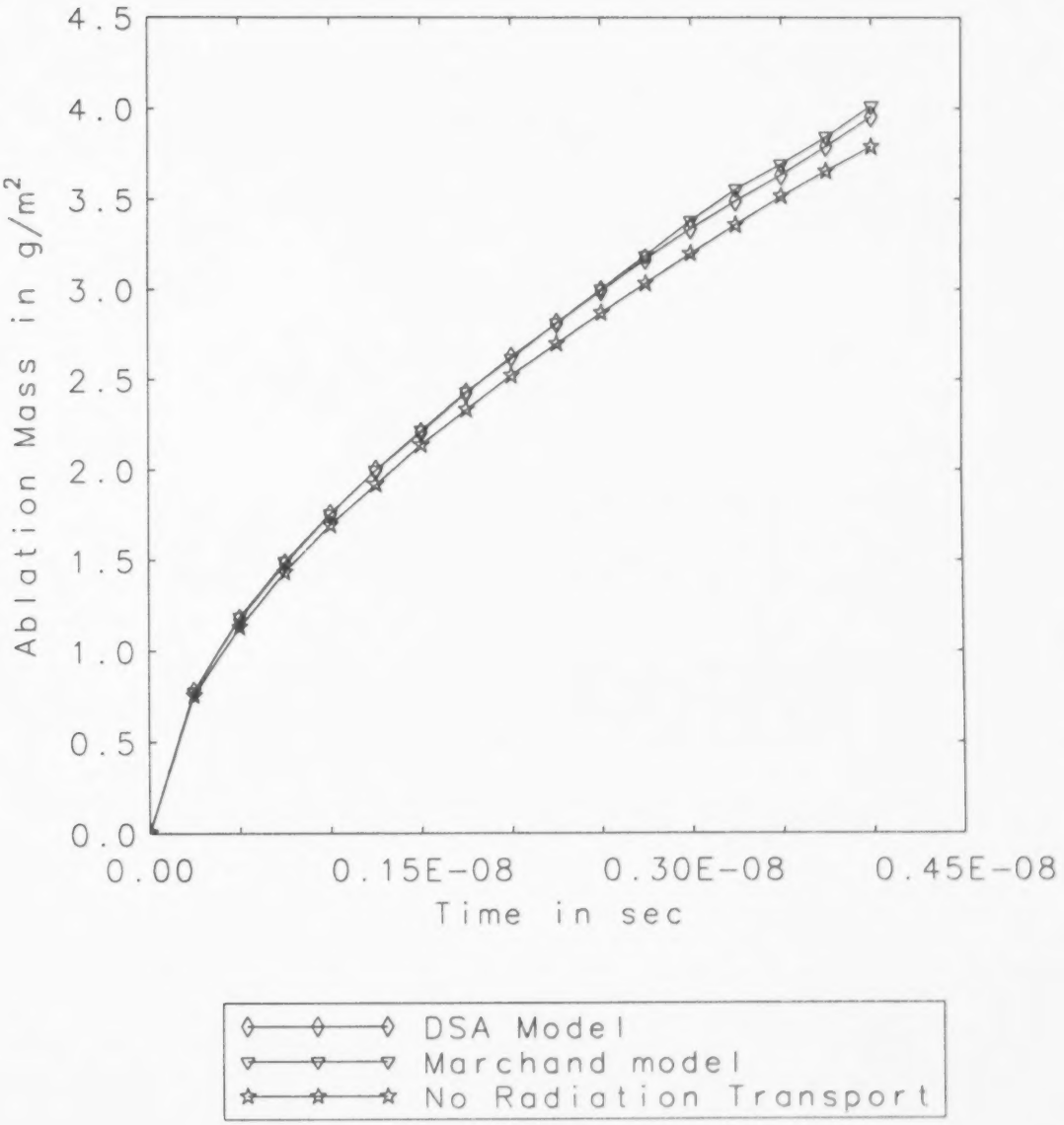

4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Ablation Mass in g/m²
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec
DSA Model
Marchand model
No Radiation Transport

Figure 5.9 b

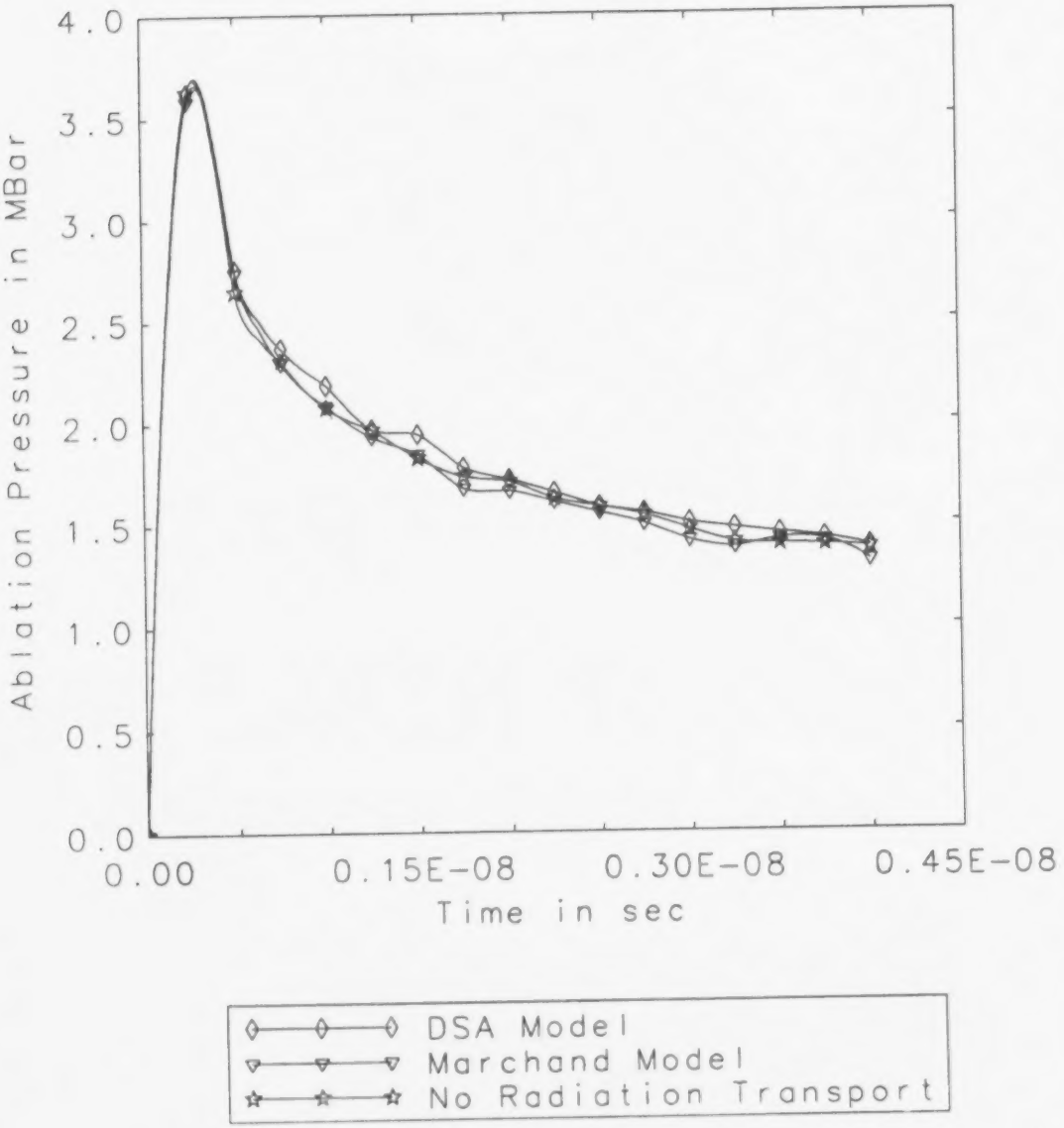

4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Ablation Pressure in MBar
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec
DSA Model
Marchand Model
No Radiation Transport

Figure 5.9 c

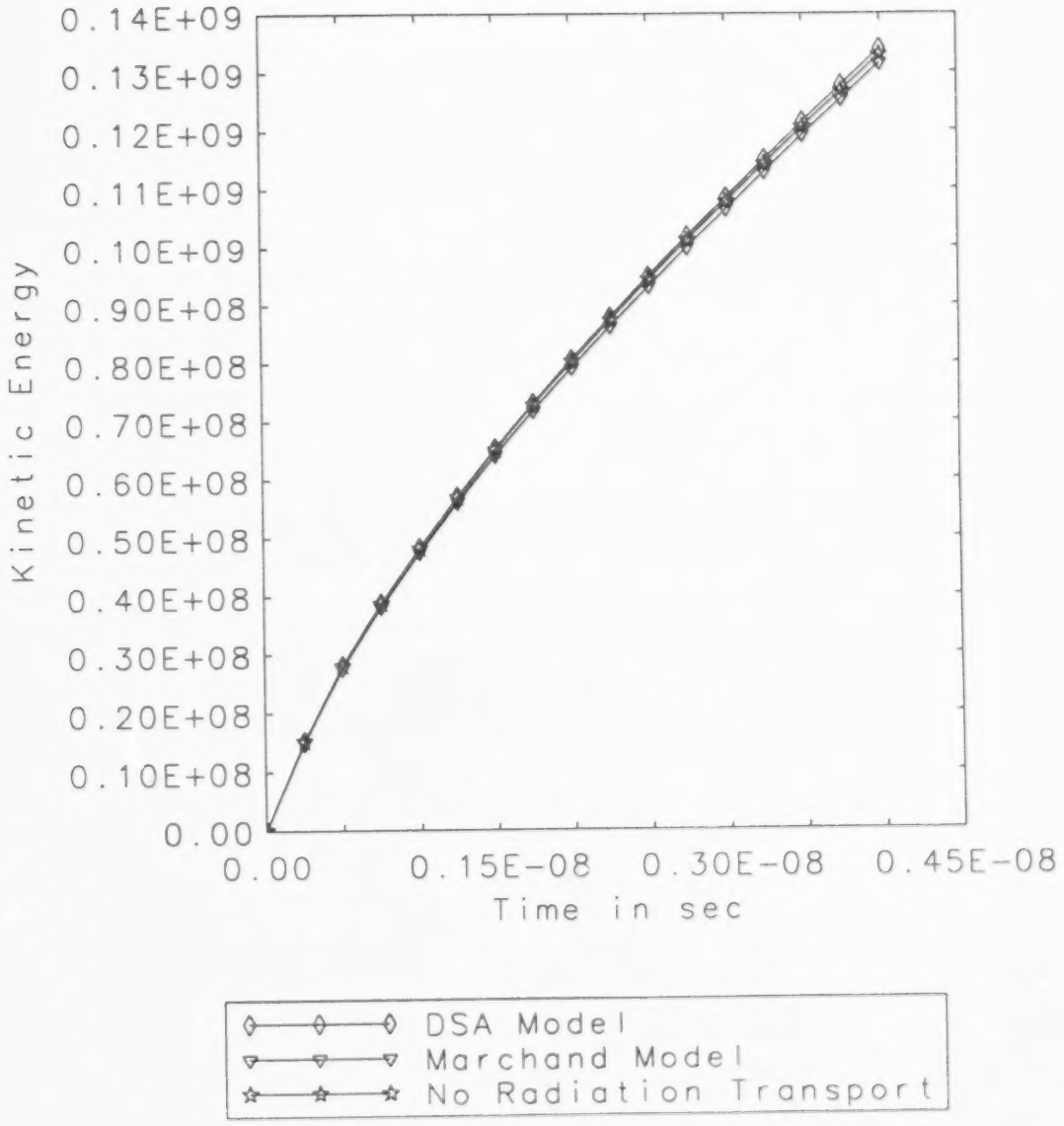

0.14E+09
0.13E+09
0.12E+09
0.11E+09
0.10E+09
0.90E+08
0.80E+08
0.70E+08
0.60E+08
0.50E+08
0.40E+08
0.30E+08
0.20E+08
0.10E+08
0.00
Kinetic Energy
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec
DSA Model
Marchand Model
No Radiation Transport

Figure 5.9 d

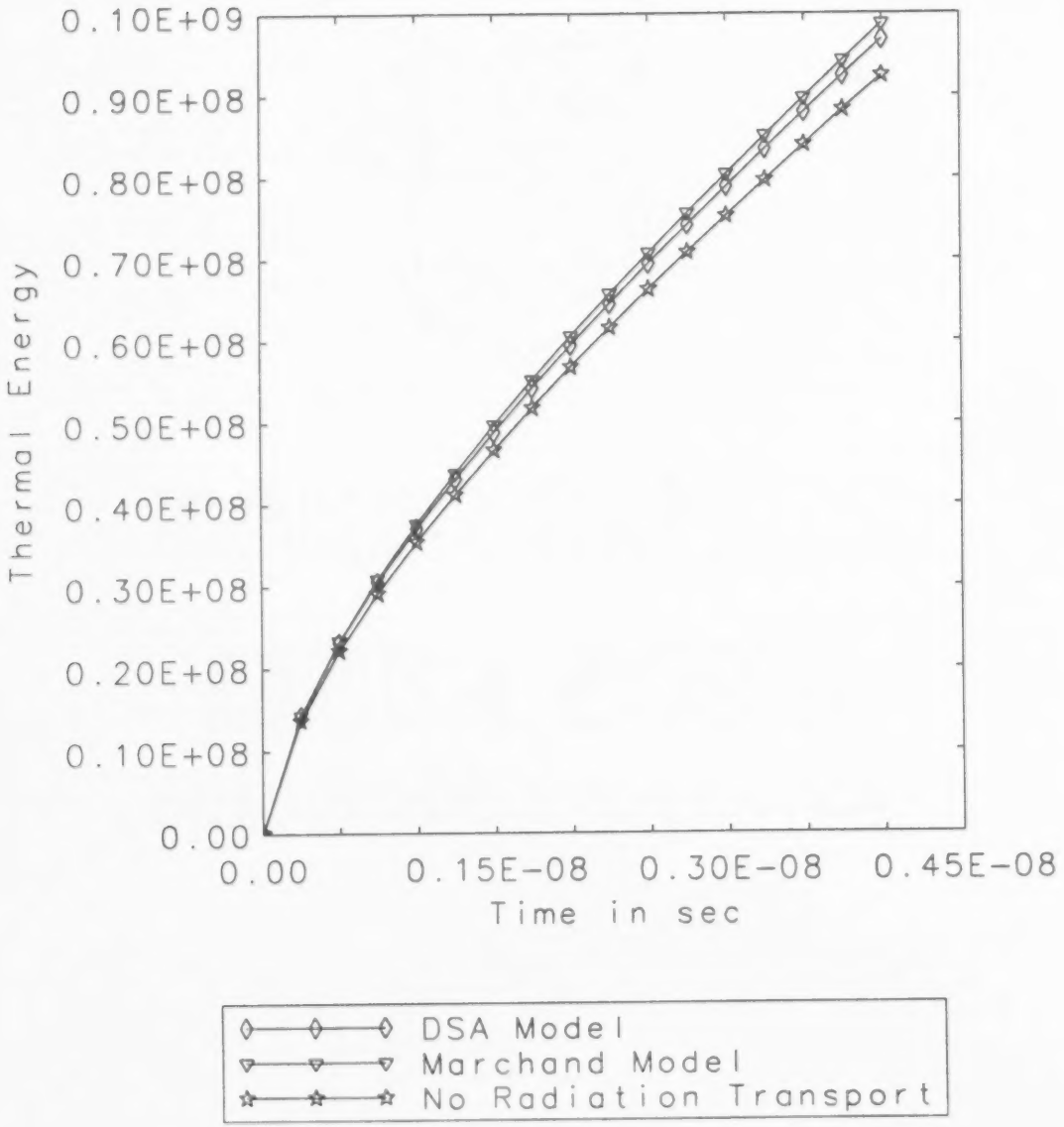
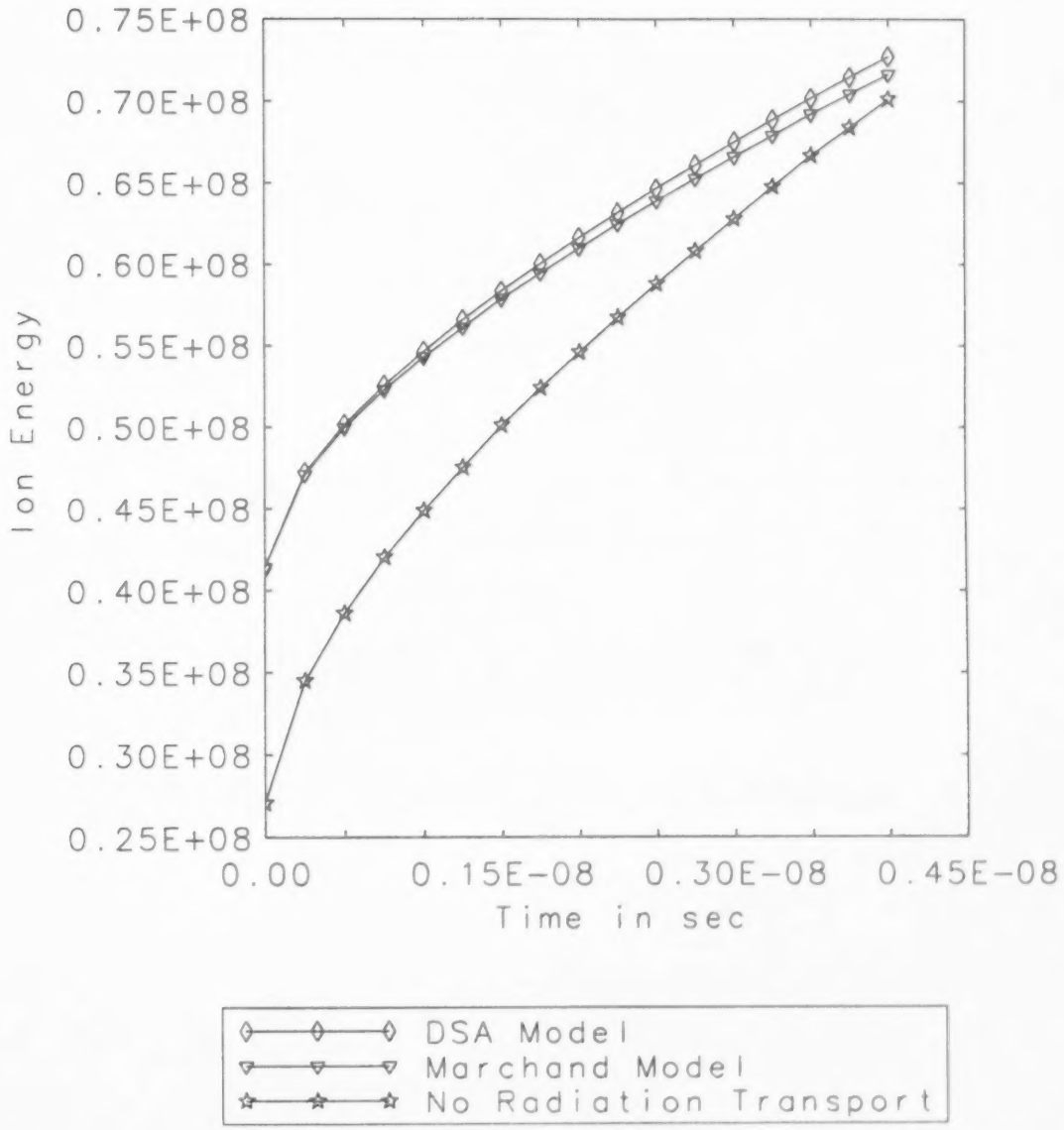
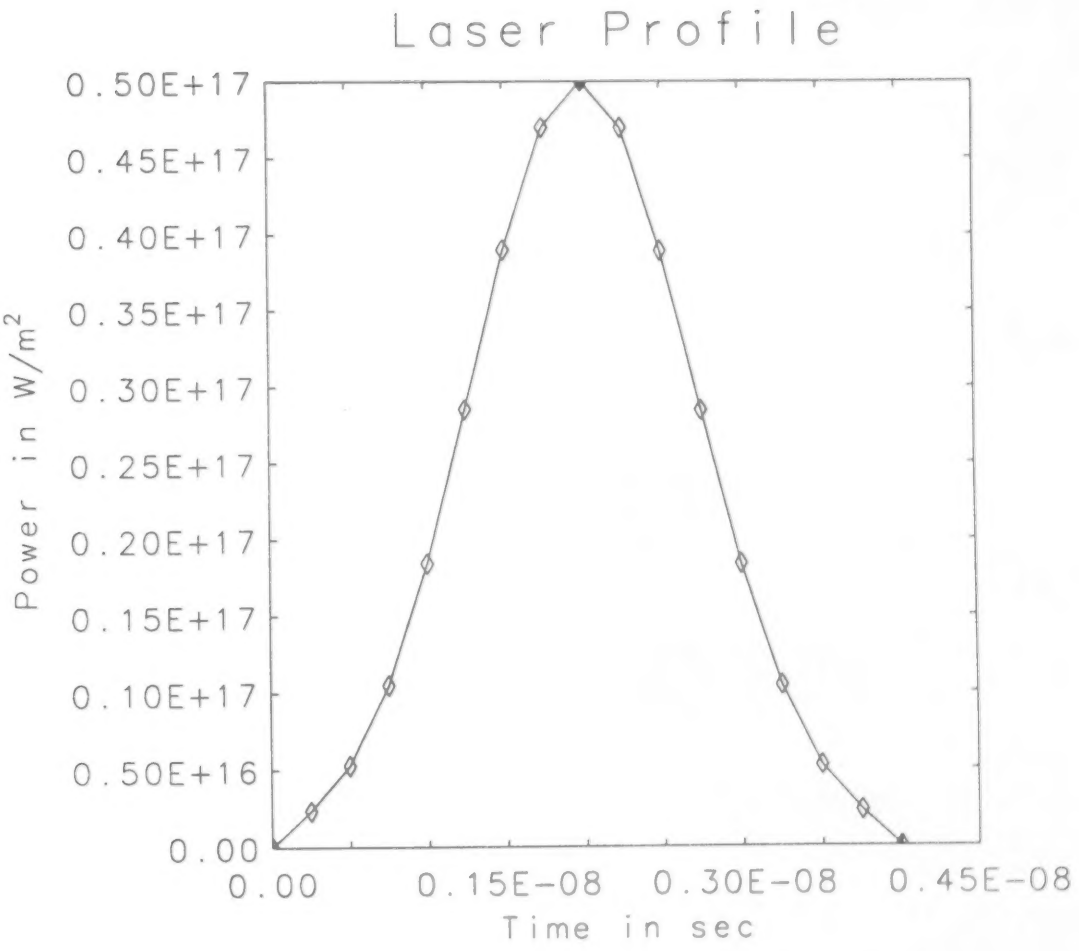

0.10E+09
0.90E+08
0.80E+08
0.70E+08
0.60E+08
0.50E+08
0.40E+08
0.30E+08
0.20E+08
0.10E+08
0.00
Thermal Energy
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec
DSA Model
Marchand Model
No Radiation Transport

Figure 5.9 e


0.75E+08
0.70E+08
0.65E+08
0.60E+08
0.55E+08
0.50E+08
0.45E+08
0.40E+08
0.35E+08
0.30E+08
0.25E+08
Ion Energy
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec
DSA Model
Marchand Model
No Radiation Transport

Laser Profile
0.35E+18
0.30E+18
0.25E+18
0.20E+18
0.15E+18
0.10E+18
0.50E+17
0.00
Power in W/m2
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec


Laser Profile
0.50E+17
0.45E+17
0.40E+17
0.35E+17
0.30E+17
0.25E+17
0.20E+17
0.15E+17
0.10E+17
0.50E+16
0.00
Power in W/m2
0.00
0.15E-08
0.30E-08
0.45E-08
Time in sec

CONCLUDING REMARKS:

The objective of the research was to solve the radiative transfer equation in one dimension by using a method that can be extended to higher dimensions or curvilinear geometries. Another objective of the research was to corroborate Marchand's simplified 2-cell model.

The Diffusion Synthetic Acceleration (**DSA**) method is chosen to solve the radiative transfer equation. This method has been successfully used to solve neutronic transport problems in higher dimensions, hence it is believed that similar extension should be possible for radiative problems. The Marshak Wave bench mark is used to test the validity of the code. It is observed that Diffusion synthetic Acceleration is very efficient compared to other methods such as SI; however, it becomes unstable at large time steps.

A comparison of DSA and Marchand's model shows that these two models give similar results when a trapezoid laser pulses are used. However, the results are not consistent when a gaussian laser beams are used. Analysis of the results shows that Marchand's model appears to give erroneous results, the ablated mass obtained with Marchand's model is unrealistic, too much mass is being ablated. Therefore, Marchand's model requires further investigation if the above error in the ablation mass is to be rectified. Marchand's model on the other hand is computationally more efficient than DSA, but its disadvantage is its applicability in only one dimensional slab geometry problems. Further, in Marchand's model the angular dependence of the intensity is ignored, which is more crucial in higher dimensions. Therefore, Marchand's model is good for nongaussian laser beams in one dimensional slab geometry, while the DSA model can be extended to higher dimensions including curvilinear geometries, though the equations involved become more complicated.

It is observed that the effects of radiation transport is more significant on the ablation mass as compared to the ablation pressure, as predicted by Mora. Inclusion of radiation transport results in an increase in thermal, kinetic and ion energy. This

is due to the fact that when radiation transport is included energy is transported as well rather than being just lost. From the simulations it appears that the increase in energy is about 7 to 10 % for kinetic, thermal and ion energies. More simulations are required to estimate the x-ray conversion efficiency and the effects of radiation transport when different wavelengths or higher intensities are used.

BIBLIOGRAPHY

1/1 A. Brueckner and Sieba Jorna; Review of Modern Physics Vol. 46, P.325, Apr 1974.
1/2 D. Duston, R.W. Clark and J. Davis; Physical Review A Vol. 31, P. 3220, May 1985.
1/3 H. Motz, Physics of Laser Fusion
1/4 R.C. Malone, R.L. McCrory and R.L. Morse; Physical Review Letter, Vol. 34, P. 721, 1975.
1/5 G.S. Fraley and R.J. Mason; Physical Review Letter, Vol. 35, P. 520, 1975.
1/6 D.W. Forslund et al; Physical Review A Vol. 11, P. 679, 1975.
1/7 E.A. McLean et al; Physical Review Letters, Vol. 45, P. 1246, 1980.
1/8 D. Duston, R.W. Clark, J. Davis and J.P. Apruzese; Physical Review Vol. A27, P. 1441, 1983.
1/9 B. Yaakobi, J. Delettrez, L.M. Goldman, R.L. McCroy, W. Seka and J.M. Soures; Optics communications Vol. 41, P. 355, May 1982.
1/10 R. Sigel et al; Physics Fluids, Vol. B2, P. 199, 1989.

2/1 G. C. Pomraning; Equations of Radiation Hydrodynamics.

3/1 Same as 2/1.
3/2 J.A. Fleck and J.D. Cummings; Journal of Computational Physics, Vol. 08, P. 313, 1971.
3/3 H.J. Kopp; Nuclear Science and Enginearing, Vol. 17, P. 65, 1964.
3/4 R.E. Alcouffe; Nuclear Sience and Enginearing, Vol. 64, P. 344, 1987.
3/5 Multiple Time Scales, Ed. J.U. Brackbill and B.I. Cohen P.74.
3/6 E.W. Larsen; Nuclear Science and Enginearing, Vol. 100, P. 255, 1988.
3/7 M.L. Adams and W.R. Martin; Nuclear Science and Enginearing, Vol. 100, P. 177, 1988.
3/8 E.D. Larsen, Personal correspondence.
3/9 Same as 2/1.
3/10 E.W. Larsen, Nuclear Science and Enginearing, Vol. 82, P. 47, 1981.
3/11 Transport and Reactor Report, Ed. R.D. O' Dell and R.E. Alcouffe, P. 29, Aug 1982.
3/12 J.E. Morel, Nuclear Science and Enginearing, Vol. 82, P. 34, 1982.
3/13 J.E. Morel, E.W. Larsen and M.K. Matzen; Journal of Quan. Spectrosc. Radiat. Transfer. Vol. 34, P. 243, 1985.

4/1 B.A. Clark; Nuclear Science and Enginearing, Vol. 90, P. 171, 1984.
4/2 R.E. Marshak; Physics of Fluids, Vol. 01, P.24, 1958.
4/3 Same as 3/5.
4/4 G. Velarde et al; Laser and Particle Beams, Vol. 7, Part 02, 305, 1989.
4/5 Same as 2/1.

5/1 Notes on MEDUSA from Dr. C.E. Capjack.
5/2 Notes on atomic tables from Dr. C.E. Capjack.
5/3 P. Mora; Physics Fluids, Vol. 25, P. 1051, 1982.
5/4 R. Marchand, R. Fedosejevs, C.E. Capjack and Y. T. Lee; Laser and Partoicle Beams, Vol. 6, Part 2, P.183, 1988.
A/1 same as 3/4.
A/2 Personal correspodance with M.L. Adams.

B/1 K. Audenaerde et al; Journal of Computational Physics Vol. 34, P. 510, 1987.
B/2 R. Marchand, A. Birnboim, C.E. Capjack and D. Salzmann; Canadian Journal of Physics, Vol. 67, P.155, 1989.
B/3 Same as 5/4.

C/1 Same as 5/2.

APPENDIX

A. NUMERICAL ASPECTS OF DSA

A.1 FOURIER ANALYSIS OF THE RADIATIVE TRANSFER EQUATION:

We start our Fourier stability analysis of the radiative transfer equation when it is discretized in time. As shown earlier in Chapter Three (3.3.12), this is given as

$$\mu\frac{\partial I}{\partial x} + (\sigma+\tau)I = \frac{\chi\eta}{2}\int_0^{\infty}\sigma I_0\, d\nu + Q$$
$$\text{where} \qquad I_0 = \int_{-1}^{1} I d\mu$$

(A.1.01)

Due to the coupling in frequency on the right hand side, we solve the above equation iteratively. The iteration strategy that is used to solve the radiative transfer equation is known as source iteration. Source iteration **(SI)** of (A.1.01) is expressed as

$$\mu\frac{\partial I^{l+\frac{1}{2}}}{\partial x} + (\sigma+\tau)I^{l+\frac{1}{2}} = \frac{\chi\eta}{2}\int_0^{\infty}\sigma I_o^{l}\, d\nu + Q$$
$$I_0^{l+1} = I_0^{l+\frac{1}{2}} = \int_{-1}^{1} I^{l+\frac{1}{2}}\, d\mu$$

(A.1.02a,b)

where the $l+1/2$ index corresponds to the most recent intensity obtained by solving (A.1.02a) with an initial intensity of I_o^l. For the next iteration, the source term (A.1.02a) is updated by using (A.1.02b). To study the convergence properties of (A.1.02), we define

$$D^{l+\frac{1}{2}} = I^{l+\frac{1}{2}} - I^{l-\frac{1}{2}} = \omega^l D\, e^{i\lambda x}$$
$$D_0^l = I_0^l - I_0^{l-1} = \omega^l D_0\, e^{i\lambda x}$$

where ω is the eigen-value and D_o is subject to the condition

$$\int_0^\infty \sigma\, D_o\, dv = 1$$

(A.1.03a,b,c)

We take σ and χ to be spatially independent for simplicity in the Fourier stability analysis. The following steps are taken to obtain the radius of convergence:

i. Write (A.1.02a) for l-1 iteration.

ii. Subtract the above equation from equations (A.1.02a) and substitute (A.1.03a,b) wherever possible.

iii. Simplify the above result using equation (A.1.03c).

iv. Repeat the first two steps for equation (A.1.02b).

Since the steps are relatively simple, only the final results are given.

$$(iii) \rightarrow (i\mu\lambda + \sigma + \tau)\, D = \frac{\chi\eta}{2}$$
$$(iv) \rightarrow \omega D_0 = \int_{-1}^{1} D\, d\mu$$

(A.1.04a,b)

The radius of convergence is obtained by manipulating (A.1.04a,b) and using (A.1.03c). The steps that are performed are as follows:

i. Multiply (A.1.04b) by σ and integrate over entire frequency spectrum

ii. Substitute (A.1.04a) into the above equation

iii. Simplify the final result by using A.1.03c

The final result after angular integration is

$$\omega = \frac{1}{2}\int_0^\infty \sigma\left[\int_{-1}^{1} \chi\eta\, \frac{d\mu}{(i\mu\lambda+\sigma+\tau)}\right] dv = \int_0^\infty \chi\eta \frac{\sigma}{\lambda} \tan^{-1}\frac{\lambda}{(\sigma+\tau)}\, dv$$

(A.1.05)

The spectral radius can be viewed as the rate at which both D and D_o go to zero, which is just the error reduction per iteration. In practice it is taken to be the largest eigen-value. In the source iteration method this occurs when $\lambda = 0$ and $\tau = 0$. When this is true the spectral radius is given by

$$spr = \int_0^\infty \chi d\nu = \eta$$

where $\eta \to 1$ when $\alpha\tau \to 0$. This is true when $\tau \to 0$ or $\sigma \gg 1$.

This result shows that the SI method can require an arbitrarily large number of iterations before a converged solution is obtained.

A.2 FOURIER ANALYSIS OF THE RADIATIVE TRANSFER EQUATION USING THE DIFFUSION EQUATION:

A Fourier stability analysis of the transfer equation when it is accelerated using the diffusion equation involves equations (3.3.12;3.3.04;3.5.02) presented earlier

$$\mu \frac{\partial I^{l+\frac{1}{2}}}{\partial x} + (\sigma+\tau) I^{l+\frac{1}{2}} = \frac{\chi\eta}{2} \int_0^\infty \sigma I_0^l \, d\nu + Q$$

$$I_0^{l+\frac{1}{2}} = \int_{-1}^{1} I^{l+\frac{1}{2}}$$

$$-\frac{1}{3(\sigma+\tau)} \frac{\partial^2 F_0^{l+1}}{\partial x^2} + (\sigma+\tau) F_0^{l+1} = \chi\eta \int_0^\infty \sigma F_0^{l+\frac{1}{2}} d\nu + \chi\eta \int_o^\infty \sigma (I_o^{l+\frac{1}{2}} - I_o^l) d\nu$$

(A.2.01;02;03)

Let us define

$$D^{l+\frac{1}{2}} = I^{l+\frac{1}{2}} - I^{l+\frac{1}{2}} = \omega^l D e^{i\alpha\lambda}$$
$$D_o^l = I_o^l - I_o^{l-1} = \omega^l D_o e^{i\alpha\lambda}$$
$$f_0^{l+1} = F_0^{l+1} - F_0^l = \omega^l f_0 \, e^{i\lambda\chi}$$
$$\text{where} \quad F_0^{l+1} = I_0^{l+1} - I_0^{l+1/2}$$

(A.2.04a,b,c,d)

A Fourier analysis of the transfer equation when accelerated with the diffusion equation involves the following steps:

i. Rewrite (A.2.01;02;03) for steps l-1, and subtract them from (A.2.01;02;03) respectively. After substituting the first equality of (A.2.04), we obtain

$$\mu \frac{\partial D^{l+\frac{1}{2}}}{\partial x} + (\sigma+\tau) D^{l+\frac{1}{2}} = \frac{\chi\eta}{2} \int_0^{\infty} \sigma D_0^l \, d\nu$$

$$D_0^{l+\frac{1}{2}} = \int_{-1}^{1} D^{l+\frac{1}{2}} \, d\mu$$

$$-\frac{1}{3(\sigma+\tau)} \frac{\partial^2 f_0^{l+1}}{\partial x^2} + (\sigma+\tau) f_0^{l+1} = \chi\eta \int_0^{\infty} \sigma f_0^{l+1} + \chi\eta \int_0^{\infty} \left[\sigma \left(\int_{-1}^{1} D^{l+\frac{1}{2}} d\mu \right) - D_0^l \right] d\nu$$

(A.2.06a,b,c)

ii. Substitute the second equality of (A.2.04) (Fourier decomposition) into (A.2.06a), to obtain

$$i\lambda\mu\omega^l \, De^{i\lambda x} + (\sigma+\tau)\omega^l De^{i\lambda x} = \frac{\chi\eta}{2} \int_o^{\infty} \omega^l D_o e^{i\lambda x} \, d\nu$$

From this we have that

$$D = \frac{\chi\eta}{2} \frac{\int_o^{\infty} D_o d\nu}{((\sigma+\tau)+i\lambda\mu)} = \frac{((\sigma+\tau)-i\lambda\mu)\chi\eta}{2} \frac{\int_o^{\infty} D_o d\nu}{((\sigma+\tau)^2+\lambda^2\mu^2)}$$

$$D_o^{l+\frac{1}{2}} = \int_{-1}^{1} \omega^l De^{i\lambda x} \, d\mu$$

$$\frac{\lambda^2}{3(\sigma+\tau)} \omega^l f_0 \, e^{i\lambda x} + (\sigma+\tau) \, \omega^l f_0 e^{i\lambda x} = \chi\eta \int_0^{\infty} \sigma \omega^l f_0 \, e^{i\lambda x} \, d\nu + \chi\eta \int_0^{\infty} \left[\sigma \int_{-1}^{1} \omega^l De^{i\lambda x} \, d\mu - \omega^l D_o e^{i\lambda x} \right] d\nu$$

After simplification the above results yields

$$\left(\frac{\lambda^2 + 3(\sigma+\tau)^2}{3(\sigma+\tau)}\right) f_o = \chi\eta \int_o^\infty \sigma f_o d\nu + \chi\eta \int_0^\infty \left[\sigma\left(\int_{-1}^{1} D d\mu\right) - D_o\right] d\nu$$

(A.2.07a,b,c,d)

iii. From (A.2.04d) we have

$$f_o^{l+1} = D_o^{l+1} - D_o^{l+\frac{1}{2}}$$
$$\omega^l f_o e^{i\lambda x} = \omega^{l+1} D_o e^{i\lambda x} - \int_{-1}^{1} D \; e^{i\lambda x} \omega^l d\mu$$
$$f_o = \omega D_o - \int_{-1}^{1} D d\mu$$

(A.2.08a,b,c)

iv. Substitute f_o in (A.2.07c) to get

$$\left(\frac{\lambda^2 + 3(\sigma+\tau)^2}{3(\sigma+\tau)}\right) \left(\omega D_0 - \int_{-1}^{1} D \, d\mu\right) = \chi\eta \int_0^\infty \left[\sigma(\omega D_0 - \int_{-1}^{1} D \, d\mu) \, d\nu\right]$$
$$+ \chi\eta \int_0^\infty \sigma \int_{-1}^{1} D d\mu d\nu - \chi\eta \int_0^\infty \sigma D_0 d\nu$$

v. Multiply the above equation by σ and divide by

$$\left(\frac{\lambda^2+3(\sigma+\tau)^2}{3(\sigma+\tau)}\right)$$

Then integrate over frequency spectrum, to obtain

$$\omega \left[\int_0^\infty \sigma D_0 d\nu - \int_0^\infty \frac{\chi\eta\sigma}{\frac{\lambda^2+3(\sigma+\tau)^2}{3(\sigma+\tau)}} \, d\nu\right] = \int_0^\infty \sigma \int_{-1}^{1} D d\mu d\nu - \int_0^\infty \left[\frac{\chi\eta\sigma}{\frac{\lambda^2+3(\sigma+\tau)^2}{3(\sigma+\tau)}}\right] d\nu$$

(A.2.09)

vi. Substitute D from (A.2.07) and use the normalization relation

$$\omega = \frac{\int_0^{\infty} \sigma \int_{-1}^{1} \chi\eta \frac{((\sigma+\tau)-i\lambda\mu)}{2((\sigma+\tau)^2+\lambda^2\mu^2)} d\mu\, dv - \int_0^{\infty} \frac{3\chi\eta\sigma(\sigma+\tau)}{(\lambda^2+3(\sigma+\tau)^2)}\, dv}{\left(1-\int_0^{\infty}\frac{3\chi\eta\sigma(\sigma+\tau)dv}{(3(\sigma+\tau)^2+\lambda^2)}\right)}$$

(A.2.10)

vii. Simplify the above equation (imaginary parts disappears after $\int d\mu$)

$$\omega = \frac{\int_{\sigma}^{\infty} \frac{\sigma\chi\eta}{2} (\sigma+\tau)dv \int_{-1}^{1}\left(\frac{1}{((\sigma+\tau)^2+\lambda^2\mu^2)} - \frac{3}{(\lambda^2+3(\sigma+\tau)^2)}\right)d\mu}{\left(1-\int_0^{\infty}\frac{3\chi\eta\sigma(\sigma+\tau)dv}{\lambda^2+3(\sigma+\tau)^2}\right)}$$

viii. After further simplification, the final result is

$$\omega = \frac{\frac{1}{2}\int_0^{\infty}\left[\frac{\sigma\chi(\sigma+\tau)}{(\lambda^2+3(\sigma+\tau)^2)}\int_{-1}^{1}\left(\frac{\lambda^2(1-3\mu^2)}{((\sigma+\tau)^2+\lambda^2\mu^2)}\right)d\mu\right]dv}{\left(1-\int_0^{\infty}\frac{3\chi\eta\sigma(\sigma+\tau)}{(\lambda^2+3(\sigma+\tau)^2)}dv\right)}$$

(A.2.11)

This shows that in the limit of $\lambda \to 0$ the spectral radius goes to zero for all values of $\tau \geq 0$. Therefore, with the solution of the diffusion equation, the solution of the transfer equation will converge rapidly even for slowly converging modes.

As stated earlier, the diffusion equation itself faces the same problem as the transfer equation, namely slow convergence. It can be shown, by using a Fourier stability analysis similar to that used for the transfer equation with SI (A.1), that the spectral radius for the diffusion equation with the source iteration technique is given by

$$\omega = \eta \int_{\sigma}^{\infty} \frac{3\sigma(\sigma+\tau)\chi}{(\lambda^2+3(\sigma+\tau)^2)}\, dv$$

$$spr = \eta\int_0^{\infty} dv \frac{\sigma\chi}{(\sigma+\tau)} \quad \to 1 \quad when \quad \tau \to 0 \ and/or \ \sigma \to \infty$$

(A.2.12)

This slow convergence can reduce the effectiveness of the diffusion equation in accelerating the transfer equation. Therefore, another equation is derived which is designed such that for slow converging modes a more rapidly converging solution is obtained. Fourier analysis is not presented here due to the complexity in its derivation, but a similar approach can be used to obtain the spectral radius of the transfer equation when it is accelerated using the diffusion equation which in turn has been accelerated by the linear grey equation.

A.3 SOLUTION OF THE RADIATIVE TRANSFER EQUATION:

We rewrite (3.4.02) here for completeness

$$\mu_m(I^{l+\frac{1}{2}}_{mgi+\frac{1}{2}} - I^{l+\frac{1}{2}}_{mgi-\frac{1}{2}}) + \sigma_{gi} I^{l+\frac{1}{2}}_{mgi} = \frac{\chi_{gi}\Delta x_i}{2}\Sigma_g \sigma_{gi} I^l_{ogi} + \Delta x_i Q_{mgi}$$

$$I^{l+\frac{1}{2}}_{mgi} = \frac{1}{2}(I^{l+\frac{1}{2}}_{mgi+\frac{1}{2}} + I^{l+\frac{1}{2}}_{mgi-\frac{1}{2}})$$

$$I^{l+1}_{ogi} = \Sigma_m I^{l+\frac{1}{2}}_{mgi}\omega_m$$

(A.3.01a,b,c)

The solution to the above equation is obtained by a so called "sweep from left to right" and then "sweep from right to left" method. The intensity incident from the left is computed independent of the intensity going to the right and vice versa.

CASE I. $\mu_m > 0$

i. Substitute (A.3.01b) for $I^{l+1/2}_{mgi+1/2}$ into (A.3.01a) and solve for $I^{l+1/2}_{mgi}$

ii. Substitute the new value for $I^{l+1/2}_{mgi}$ in (A.3.01b) to obtain $I^{l+1/2}_{mgi+1/2}$ which will be used as $I^{l+1/2}_{mgi-1/2}$ for the next cell, and so on.

iii. If $I^{l+1/2}_{mgi+1/2}$ is less than zero, let $I^{l+1/2}_{mgi+1/2}=0$ or $I^{l+1/2}_{mgi+1/2}=I^{l+1/2}_{mgi}$ in (A.3.01) and solve again for $I^{l+1/2}_{mgi}$

CASE II. $\mu_m < 0$

The procedure is the same as for $\mu_m > 0$ except that $I^{l+1/2}_{mgi\pm1/2}$ is replaced by

$I^{l+1/2}_{mgi+1/2}$.

For the next iteration, $I^{l+1/2}_{mgi}$ obtained from (A.3.01b) is used to get the new source term for (A.3.01a). The final set of equations for $\mu_m > 0$ is given as

$$I^{l+\frac{1}{2}}_{mgi} = \frac{\left[\frac{\chi_{gi}\eta_i\Delta x_i}{2}\ \Sigma_g\ \sigma_{gi}I^{l}_{ogi} + \Delta x_i\ Q_{mgi} + 2\mu_m I^{l+\frac{1}{2}}_{mgi-\frac{1}{2}}\right]}{(\hat{\sigma}_{gi} + 2\mu_m)}$$

$$I^{l+\frac{1}{2}}_{mgi+\frac{1}{2}} = 2\, I^{l+\frac{1}{2}}_{mgi} - I^{l+\frac{1}{2}}_{mgi-\frac{1}{2}}$$

If $I^{l+1/2}_{mgi}$ is negative then, according to a parameter ξ $(=c\Delta t/\Delta x)$

$$\xi < 1 \qquad I^{l+\frac{1}{2}}_{mgi} = \frac{\left[\frac{\chi_{gi}\eta_i\Delta x_i}{2}\ \Sigma_g\sigma_{gi}I^{1}_{ogi} + \Delta x_i Q_{mgi} + \mu_m I^{1+\frac{1}{2}}_{mgi-\frac{1}{2}}\right]}{\hat{\sigma}_{gi}}$$

$$I^{l+\frac{1}{2}}_{mgi+\frac{1}{2}} = 0.0$$

$$\xi \geq 1 \qquad I^{1+\frac{1}{2}}_{mgi} = \frac{\left[\frac{\chi_{gi}\eta_i\Delta x_i}{2}\ \Sigma_g\sigma_{gi}I^{1}_{ogi} + \Delta x_i Q_{mgi} + \mu_m I^{1+\frac{1}{2}}_{mgi-\frac{1}{2}}\right]}{(\hat{\sigma}_{gi} + \mu_m)}$$

$$I^{l+\frac{1}{2}}_{mgi+\frac{1}{2}} = I^{l+\frac{1}{2}}_{mgi}$$

(A.3.02a,b;03a,b;04a,b)

If $\mu_m < 0$,

$$I^{l+\frac{1}{2}}_{mgi} = \frac{\left[\frac{\chi_{gi}\eta_i\Delta x_i}{2}\ \Sigma_g\ \sigma_{gi}I^{l}_{ogi} + \Delta\chi_i\ Q_{mgi} - 2\mu_m I^{l+\frac{1}{2}}_{mgi+\frac{1}{2}}\right]}{(\hat{\sigma}_{gi} - 2\mu_m)}$$

$$I^{l+\frac{1}{2}}_{mgi-\frac{1}{2}} = 2\, I^{l+\frac{1}{2}}_{mgi} - I^{l+\frac{1}{2}}_{mgi+\frac{1}{2}}$$

If $I^{l+1/2}_{mgi}$ is negative then,

$$\xi < 1 \qquad I_{mgi}^{l+\frac{1}{2}} = \frac{\left[\frac{\chi_{gi}\eta_i\Delta x_i}{2}\,\Sigma_g\sigma_{gi}I_{ogi}^{1} + \Delta x_i Q_{mgi} - \mu_m I_{mgi-\frac{1}{2}}^{l+\frac{1}{2}}\right]}{\hat{\sigma}_{gi}}$$

$$I_{mgi-\frac{1}{2}}^{l+\frac{1}{2}} = 0.0$$

$$\xi \geq 1 \qquad I_{mgi}^{l+\frac{1}{2}} = \frac{\left[\frac{\chi_{gi}\eta_i\Delta x_i}{2}\,\Sigma_g\sigma_{gi}I_{ogi}^{1} - \Delta x_i Q_{mgi} + \mu_m I_{mgi-\frac{1}{2}}^{l+\frac{1}{2}}\right]}{(\hat{\sigma}_{gi} - \mu_m)}$$

$$I_{mgi-\frac{1}{2}}^{l+\frac{1}{2}} = I_{mgi}^{l+\frac{1}{2}}$$

(A.3.05a,b;06a,b;07a,b)

The new source term is obtained by summing the new specific intensity from the transfer equation as

$$I_{ogi}^{l+1} = I_{ogi}^{l+\frac{1}{2}} = \Sigma_m\, I_{mgi}^{l+\frac{1}{2}}\,\omega_m$$

(A.3.08)

Therefore, one complete solution of the transfer equation with source iteration can involve equations (A.3.03;04;05;06;07;08).

A.4 DERIVATION OF DISCRETIZED FORM OF THE DIFFUSION EQUATION:

In order to obtain a diffusion equation which is consistent with the transfer equation just solved, one must start with (3.5.02) instead of (3.3.12). Alcouffe showed[A/1] that the diffusion obtain equation from (3.7.27) leads to unstable solutions. The following steps are taken in order to obtain the discretized diffusion equation from the transfer equation.

i. Multiply equation (A.3.01) by ω_m and $\omega_m\mu_m$ and sum over the angular space to obtain the zeroth and first order moment in angular

space. This yields

$$(I^{l+\frac{1}{2}}_{1gi+\frac{1}{2}} - I^{l+\frac{1}{2}}_{1gi-\frac{1}{2}}) + \hat{\sigma}_{gi}\, I^{l+\frac{1}{2}}_{ogi} = \chi_{gi}\eta_l \Delta x_l \Sigma_g \sigma_{gi} I^{l}_{ogi} + \Delta x_l Q_{ogi}$$

$$\frac{2}{3}(I^{l+\frac{1}{2}}_{2gi+\frac{1}{2}} - I^{l+\frac{1}{2}}_{2gi-\frac{1}{2}}) + \frac{1}{3}(I^{l+\frac{1}{2}}_{ogi+\frac{1}{2}} - I^{l+\frac{1}{2}}_{ogi-\frac{1}{2}}) + \hat{\sigma}_{gi} I^{l+\frac{1}{2}}_{1gi} = Q_{1gi}\Delta x_l$$

(A.4.01;02)

Here we used the facts that

$$I^{l+\frac{1}{2}}_{2gi} = \Sigma_m\, I^{l+\frac{1}{2}}_{mgi}\, \omega_m \left(\frac{3\mu_m^2 - 1}{2}\right) = \frac{3}{2}\,\Sigma\, \mu_m^2\, \omega_m\, I^{l+\frac{1}{2}}_{mgi} - \frac{1}{2}\, I^{l+\frac{1}{2}}_{ogi}$$

$$\Sigma_m\, \omega_m \mu_m = 0$$

$$Q_{ogi} = \frac{\chi_{gi}\, \eta_l\, \mu_s^n}{\beta_l \Delta t^n} + \tau^n\, I^n_{ogi}$$

$$Q_{1gi} = \tau^n I_1 gi$$

(A.4.04a,b,c)

ii. The accelerated form of the diffusion equation is obtained by accelerating only the first two moments, as given below

$$(I^{l+1}_{1gi+\frac{1}{2}} - I^{l+1}_{1gi-\frac{1}{2}}) + \hat{\sigma}_{gi}\, I^{l+1}_{ogi} = \chi_{gi}\, \eta_l\, \Delta x_l\, \Sigma_g\, \sigma_{gi}\, I^{l+1}_{ogi} + \Delta x_l\, Q_{ogi}$$

$$\frac{2}{3}(I^{l+\frac{1}{2}}_{2gi+\frac{1}{2}} - I^{l+\frac{1}{2}}_{2gi-\frac{1}{2}}) + \frac{1}{3}(I^{l+1}_{ogi+\frac{1}{2}} - I^{l+1}_{ogi-\frac{1}{2}}) + \hat{\sigma}_{gi}\, I^{l+1}_{1gi} = Q_{1gi}\Delta x_l$$

(A.4.05;06)

The DD relationship is redefined in order to eliminate the instability due to the negative flux fix up in the transfer equation, as

$$I_{ngi}^{l+1} = \frac{1}{2}\left[a_{ogi}\, I_{ogi+\frac{1}{2}}^{l+1} + b_{ogi}\, I_{ogi-\frac{1}{2}}^{l+1}\right] \qquad n = 0,1$$

(A.4.07)

where the choice of a_{ogi} and b_{ogi} is somewhat based on trial and error approach.

To obtain the diffusion equation in the form of a tridiagonal matrix, the following manipulative steps are taken

i. Equate (A.4.02) and (A.4.06).

ii. Substitute (A.4.07) in it for n=1 with $a_{1gi} = b_{1gi} = 1$.

iii. Write the resultant for i+1.

iv. Divide (ii) and (iii) by σ_{gi} and σ_{gi+1} respectively.

v. Eliminate (A.4.05) for $I^{l+1}{}_{1gi-1/2}$.

vi. Rewrite (A.4.05) for i=i+1 and eliminate for $I^{l+1/2}{}_{1gi+3/2}$.

vii. Substitute $I^{l+1}{}_{1gi-1/2}$ and $I^{l+1}{}_{1gi+3/2}$ from v and vi into step iv.

viii. Substitute (A.4.07) for n=0 in (vii) .

ix. Subtract the resulting two equation from the two equations obtained in step vii.

The final result is

$$\begin{aligned}
&-\frac{1}{3\hat{\sigma}_{gi+1}}\left[I_{ogi+\frac{3}{2}}^{l+1} - I_{ogi+\frac{1}{2}}^{l+1}\right] + \frac{1}{3\hat{\sigma}_{gi}}\left[I_{ogi+\frac{1}{2}}^{l+1} - I_{ogi-\frac{1}{2}}^{l+1}\right] \\
&+ \frac{\hat{\sigma}_{gi+1}}{4}\left[a_{ogi+1} I_{ogi+\frac{3}{2}}^{l+1} + b_{ogi+1} I_{ogi+\frac{1}{2}}^{l+1}\right] + \frac{\hat{\sigma}_{gi}}{4}\left[a_{ogi} I_{ogi+\frac{1}{2}}^{l+1} + b_{ogi} I_{ogi-\frac{1}{2}}^{l+1}\right] \\
&= \frac{1}{4}\left[\chi_{gi+1}\eta_{i+1}\Delta x_{i+1}\Sigma_g\ \sigma_{gi+1}(a_{0gi+1} I_{0gi+\frac{3}{2}}^{l+1} + b_{0gi+1} I_{0gi+\frac{1}{2}}^{l+1})\right] \\
&+ \frac{1}{4}\left[\chi_{gi}\eta_i\Delta x_i\Sigma_g\ \sigma_{gi}(a_{0gi} I_{0gi+\frac{1}{2}}^{l+1} + b_{0gi} I_{0gi-\frac{1}{2}}^{l+1})\right] + S_{gi}^{l+\frac{1}{2}}
\end{aligned}$$

(A.4.08)

Where $S_{gi}^{l+1/2}$ consists of variables which do not change during iteration of the diffusion equation, and is given as

$$S_{gi}^{l+\frac{1}{2}} = \frac{\Delta x_i\, Q_{0gi}}{2} + \frac{\Delta x_{i+1}\, Q_{0gi+1}}{2} - \frac{1}{3\hat{\sigma}_{gi+1}}\left[I_{ogi+\frac{3}{2}}^{l+\frac{1}{2}} - I_{ogi+\frac{1}{2}}^{l+\frac{1}{2}}\right] + \frac{1}{3\hat{\sigma}_{gi}}\left[I_{ogi+\frac{1}{2}}^{l+\frac{1}{2}} - I_{ogi-\frac{1}{2}}^{l+\frac{1}{2}}\right] - \frac{1}{2}\left[I_{1gi+\frac{3}{2}}^{l+\frac{1}{2}} - I_{1gi-\frac{1}{2}}^{l+\frac{1}{2}}\right]$$

(A.4.09)

A.5 DERIVATION OF THE DISCRETIZED FORM OF THE GREY EQUATION:

A discretized form of the diffusion equation was obtained from the discretized transfer equation to ensure stability. The grey diffusion equation is derived from the discretized form of the diffusion equation, namely equation (A.4.08).

The accelerated form of the diffusion equation is obtained by summing the frequency groups with a particular weight function. The following substitution is made in (A.4.08) before summing over the frequency groups in order to obtain the grey equation.

Consider the following transformation to be used in the diffusion equation

$$f_{gi}^{k^*} = (a_{ogi} I^{k^*}_{ogi+\frac{1}{2}} + b_{ogi} I^{k^*}_{ogi-\frac{1}{2}}) - \theta_{gi}^{k+\frac{1}{2}} (a_{oi} I^{k+1}_{oi+\frac{1}{2}} + b_{oi} I^{k+1}_{oi-\frac{1}{2}}) + f_{gi}^{k+\frac{1}{2}} - \theta_{gi}^{k+\frac{1}{2}} (a_{oi} I^{k+\frac{1}{2}}_{oi+\frac{1}{2}} + b_{oi} I^{k+\frac{1}{2}}_{oi-\frac{1}{2}})$$

$$g_{gi}^{k+\frac{1}{2}} = (I^{k+\frac{1}{2}}_{ogi+\frac{1}{2}} - I^{k+\frac{1}{2}}_{ogi-\frac{1}{2}}) - \varphi_{gi}^{k+\frac{1}{2}} (I^{k+1}_{oi+\frac{1}{2}} - I^{k+1}_{oi-\frac{1}{2}}) + g_{gi}^{k+\frac{1}{2}} - \varphi_{gi}^{k+\frac{1}{2}} (I^{k+\frac{1}{2}}_{oi+\frac{1}{2}} - I^{k+\frac{1}{2}}_{oi-\frac{1}{2}})$$

(A.5.01a,b)

$$a_{\alpha i} = \frac{\Sigma_g (a_{\alpha g i} I^{k+\frac{1}{2}}_{\alpha g i+\frac{1}{2}})}{I^{k+\frac{1}{2}}_{\alpha i+\frac{1}{2}}}, \quad b_{\alpha i} = \frac{\Sigma_g (b_{\alpha g i} I^{k+\frac{1}{2}}_{\alpha g i-\frac{1}{2}})}{I^{k+\frac{1}{2}}_{\alpha i-\frac{1}{2}}}, \quad I^{k+\frac{1}{2}}_{\alpha i+\frac{1}{2}} = \Sigma_g I^{k+\frac{1}{2}}_{\alpha g i+\frac{1}{2}}$$

(A.5.02a,b,c)

k^* can be k or $k+1/2$ corresponding to values before and after acceleration. The resultant equation is

$$
\begin{aligned}
&- \Sigma_g \frac{1}{3\hat{\sigma}_{gi+1}} \left[\varphi^{k+1/2}_{gi+1} \left(I^{k+1}_{\alpha i+\frac{3}{2}} - I^{k+1}_{\alpha i+\frac{1}{2}} \right)^{\#1} + \left(I^{k+\frac{1}{2}}_{\alpha g i+\frac{3}{2}} - I^{k+\frac{1}{2}}_{\alpha g i+\frac{1}{2}} \right)^{\#2} - \varphi^{k+1/2}_{gi+1} \left(I^{k+\frac{1}{2}}_{\alpha i+\frac{3}{2}} - I^{k+\frac{1}{2}}_{\alpha i+\frac{1}{2}} \right)^{\#3} \right] \\
&+ \Sigma_g \frac{1}{3\hat{\sigma}_{gi}} \left[\varphi^{k+1}_{gi} \left(I^{k+1}_{\alpha i+\frac{1}{2}} - I^{k+1}_{\alpha i-\frac{1}{2}} \right)^{\#4} + \left(I^{k+\frac{1}{2}}_{\alpha g i+\frac{1}{2}} - I^{k+\frac{1}{2}}_{\alpha i-\frac{1}{2}} \right)^{\#5} - \varphi^{k+\frac{1}{2}}_{gi} \left(I^{k+\frac{1}{2}}_{\alpha i+\frac{1}{2}} - I^{k+\frac{1}{2}}_{\alpha i-\frac{1}{2}} \right)^{\#6} \right] \\
&+ \Sigma_g \frac{\hat{\sigma}_{gi+1}}{4} \left[\theta^{k+1/2}_{gi+1} \left(a_{\alpha i+1} I^{k+1}_{\alpha i+\frac{3}{2}} + b_{\alpha i+1} I^{k+1}_{\alpha i+\frac{1}{2}} \right)^{\#7} + f^{k+\frac{1}{2}^{\#8}}_{gi+1} - \theta^{k+\frac{1}{2}}_{gi+1} \left(a_{\alpha i+1} I^{k+\frac{1}{2}}_{\alpha i+\frac{3}{2}} + b_{\alpha i+1} I^{k+\frac{1}{2}}_{\alpha i+\frac{1}{2}} \right)^{\#9} \right] \\
&+ \Sigma_g \frac{\hat{\sigma}_{gi}}{4} \left[\theta^{k+\frac{1}{2}}_{gi} \left(a_{\alpha i} I^{k+1}_{\alpha g i+\frac{1}{2}} + b_{\alpha i} I^{k+1}_{\alpha g i-\frac{1}{2}} \right)^{\#10} + f^{k+\frac{1}{2}^{\#11}}_{gi} - \theta^{k+\frac{1}{2}}_{gi} \left(a_{\alpha i} I^{k+\frac{1}{2}}_{\alpha i+\frac{1}{2}} + b_{\alpha i} I^{k+\frac{1}{2}}_{\alpha i-\frac{1}{2}} \right)^{\#12} \right] \\
&= \Sigma_g \frac{1}{4} \chi_{gi+1} \eta_{l+1} \Delta x_l \Sigma_g \sigma_{gi+1} \left[\theta^{k+1/2}_{gi+1} \left(a_{\alpha i+1} I^{k+1}_{\alpha i+\frac{3}{2}} + b_{\alpha i+1} I^{k+1}_{\alpha i+\frac{1}{2}} \right)^{\#13} + f^{k+1/2^{\#14}}_{gi+1} - \theta^{k+\frac{1}{2}}_{gi+1} \left(a_{\alpha i+1} I^{k+\frac{1}{2}}_{\alpha i+\frac{3}{2}} + b_{\alpha i+1} I^{k+1/2}_{\alpha i+\frac{1}{2}} \right)^{\#15} \right] \\
&+ \Sigma_g \frac{1}{4} \chi_{gi} \eta_l \Delta x_l \Sigma_g \sigma_{ogi} \left[\theta^{k+\frac{1}{2}}_{ogi} \left(a_{\alpha i} I^{k+\frac{1}{2}}_{\alpha i+\frac{1}{2}} + b_{\alpha i} I^{k+\frac{1}{2}}_{\alpha i-\frac{1}{2}} \right)^{\#16} + f^{k+\frac{1}{2}^{\#17}}_{gi} - \theta^{k+\frac{1}{2}}_{gi} \left(a_{\alpha i} I^{k+\frac{1}{2}}_{l+\frac{1}{2}} + b_{\alpha i} I^{k+\frac{1}{2}}_{\alpha i-\frac{1}{2}} \right)^{\#18} \right] \\
&+ \Sigma_g S^{l+\frac{1}{2}^{\#19}}_{gi}
\end{aligned}
$$

(A.5.04)

These relations simply reflect that a correction term is added to both sides of (A.4.08) in order that the accelerated form of the new equation yields the solution more rapidly by projecting out the slow converging modes. Before the final form of the Grey equation is presented, consider the following manipulative steps taken to obtain the final form of the grey equation.

Suppose we have an arbitrary function ψ_g which is a function of frequency and space. Consider the two terms (#7 & #13) from (A.5.04)

$$\Sigma_g \left[\dot{o}_{gi}\ \psi_{gi} - \Delta x_i\ \chi_{gi}\ \eta_i\ \Sigma_g\ \sigma_g \psi_{gi}\right]$$

where other variables are as previously defined

$$= \Sigma_g \left[\ (\sigma_{gi} + \tau)\Delta x_i\ \psi_{gi} - \Delta x_i\ \chi_{gi}\ \eta_i\ \Sigma_g\ \sigma_{gi}\ \psi_{gi}\right]$$

$$= \Sigma_g \left[\ \sigma_{gi}\ \Delta x_i + \tau \Delta x_i - \frac{\Delta x_i\ \chi_{gi}}{(1+\alpha_i \tau)}\ \Sigma_g\ \sigma_{gi}\right]\psi_{gi}$$

$$= \Sigma_g \left[\ \sigma_{gi}\ \Delta x_i + \tau \Delta x_i - \frac{\Delta x_i \sigma_{gi}}{(1+\alpha_i \tau)}\ \Sigma_g\ \chi_{gi}\right]\psi_{gi}$$

$$= \Sigma_g \left[\ \dot{o}_{gi}\ \psi_{gi} - \Delta x_i \chi_{gi} \eta_i \Sigma_g \sigma_{gi} \psi_{gi}\right]$$

$$= \Sigma_g \left[\tau \Delta x_i + \frac{\alpha_i \sigma_{gi} \tau \Delta x_i}{(1+\alpha_i \tau)}\right]\psi_{gi}$$

$$= \Sigma_g \left[1 + \alpha_i \sigma_{gi} \eta_i\right]\psi_{gi} \tau \Delta x_i$$

let $\xi_{gi} = (1+\alpha_i \sigma_{gi} \eta_i)\tau \Delta x_i$

(A.5.05)

If ψ_{gi} is taken to be $\theta^{k+1/2}$,then above result can be written as

$$\xi_i = \Sigma_g\ \xi_{gi}\ \theta_{gi}^{k+\frac{1}{2}}$$

With the above manipulation and keeping only k+1 terms on left side of equation (A.5.04), it reduces to

$$
\begin{aligned}
&- \sum_g \frac{\varphi_{gi+1}^{k+\frac{1}{2}}}{3\hat{\sigma}_{gi+1}}\left(I_{\alpha i+\frac{3}{2}}^{k+1} - I_{\alpha i+\frac{1}{2}}^{k+1}\right) + \sum_g \frac{\varphi_{gi}^{k+\frac{1}{2}}}{3\hat{\sigma}_{gi}}\left(I_{\alpha i+\frac{1}{2}}^{k+1} - I_{\alpha i-\frac{1}{2}}^{k+1}\right) \\
&+ \frac{\xi_{i+1}}{4}\left(a_{\alpha i+1} I_{\alpha i+\frac{3}{2}}^{k+1} + b_{\alpha i+1} I_{\alpha i+\frac{1}{2}}^{k+1}\right) + \frac{\xi_i}{4}\left(a_{\alpha i} I_{\alpha i+\frac{1}{2}}^{k+1} + b_{\alpha i} I_{\alpha i-\frac{1}{2}}^{k+1}\right) \\
&= \sum_g \left[\frac{1}{3\hat{\sigma}_{gi+1}}\left(I_{\alpha gi+\frac{3}{2}}^{k+\frac{1}{2}} - I_{\alpha gi+\frac{1}{2}}^{k+\frac{1}{2}}\right) - \frac{1}{3\hat{\sigma}_{gi}}\left(I_{\alpha gi+\frac{1}{2}}^{k+\frac{1}{2}} - I_{\alpha gi-\frac{1}{2}}^{k+\frac{1}{2}}\right)\right] \\
&- \sum_g \left[\frac{\varphi_{gi+1}^{k+\frac{1}{2}}}{3\hat{\sigma}_{gi+1}}\left(I_{\alpha i+\frac{3}{2}}^{k+\frac{1}{2}} - I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}}\right) - \frac{\varphi_{gi}^{k+\frac{1}{2}}}{3\hat{\sigma}_{gi}}\left(I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}} - I_{\alpha i-\frac{1}{2}}^{k+\frac{1}{2}}\right)\right] \\
&- \frac{1}{4}\sum_g \left(\xi_{gi+1} f_{gi+1}^{k+\frac{1}{2}} + \xi_{gi} f_{gi}^{k+\frac{1}{2}}\right) \\
&+ \frac{1}{4}\left[\xi_{i+1}\left(a_{\alpha i+1} I_{\alpha i+\frac{3}{2}}^{k+\frac{1}{2}} + b_{\alpha i+1} I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}}\right) + \xi_i\left(a_{\alpha i} I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}} + b_{\alpha i} I_{\alpha i-\frac{1}{2}}^{k+\frac{1}{2}}\right)\right] \\
&+ \sum_g S_{gi}^{k+\frac{1}{2}}
\end{aligned}
$$

(A.5.06)

The solution of the grey equation depends on the choice of the spectral functions θ and φ. One expression for θ and φ corresponds to the spectral function causing slowest convergence. In this case θ and φ are taken to be same and are given as

$$
\theta_{gi}^{k+\frac{1}{2}} = \varphi_{gi}^{k+\frac{1}{2}} = \frac{\chi_{gi}/(\sigma_{gi}+\tau)}{\Sigma_g[\chi_{gi}/(\sigma_{gi}+\tau)]}
$$

(A.5.07)

This is known as the linear case. The other expression for θ and φ is known as the non linear case and is given as

$$
\theta_{gi}^{k+\frac{1}{2}} = \frac{f_{gi}^{k+\frac{1}{2}}}{\left(a_{\alpha i} I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}} + b_{\alpha i} I_{\alpha i-\frac{1}{2}}^{k+\frac{1}{2}}\right)}, \quad \varphi_{gi}^{k+\frac{1}{2}} = \frac{g_{gi}^{k+\frac{1}{2}}}{\left(I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}} - I_{\alpha i-\frac{1}{2}}^{k+\frac{1}{2}}\right)}
$$

(A.5.08a,b)

When the nonlinear expression is substituted in (A.5.06), it reduces to

$$- \Sigma_g \frac{1}{3\hat{\sigma}_{gi+1}} \left[\varphi_{gi+1}^{k+\frac{1}{2}} \left(I_{\alpha i+\frac{3}{2}}^{k+1} - I_{\alpha i+\frac{1}{2}}^{k+1} \right) \right] + \Sigma_g \frac{1}{3\hat{\sigma}_{gi}} \left[\varphi_{gi}^{k+\frac{1}{2}} \left(I_{\alpha i+\frac{1}{2}}^{k+1} - I_{gi-\frac{1}{2}}^{k+1} \right) \right]$$
$$+ \frac{1}{4} \left[\xi_{i+1} \left(a_{\alpha i+1} I_{\alpha i+\frac{3}{2}}^{k+1} + b_{\alpha i+1} I_{\alpha gi+\frac{1}{2}}^{k+1} \right) \right] + \frac{1}{4} \left[\xi_i \left(a_{\alpha i} I_{\alpha i+\frac{1}{2}}^{k+1} + b_{\alpha i} I_{\alpha i-\frac{1}{2}}^{k+1} \right) \right] = \Sigma_g S_{gi}^{i+\frac{1}{2}}$$

(A.5.09)

The following steps are utilized to obtain above equation. Consider the following expression from right side of (A.5.06)

$$\Sigma_g \frac{\varphi_{gi}^{k+\frac{1}{2}}}{\hat{\sigma}_{gi}} (I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}} - I_{\alpha i-\frac{1}{2}}^{k+\frac{1}{2}}) + \xi_i (a_{\alpha i} I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}} - b_{\alpha i} I_{\alpha i-\frac{1}{2}}^{k+\frac{1}{2}})$$

(A.5.10)

If we substitute the nonlinear expression (A.5.08a,b) in (A.5.10)

$$\sum_g \frac{1}{\hat{\sigma}_{gi}} \frac{(I_{\alpha gi+\frac{1}{2}}^{k+\frac{1}{2}} - I_{\alpha gi-\frac{1}{2}}^{k+\frac{1}{2}})(I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}} - I_{\alpha i-\frac{1}{2}}^{k+\frac{1}{2}})}{(I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}} - I_{\alpha i-\frac{1}{2}}^{k-\frac{1}{2}})}$$
$$+ \sum_g \left[\frac{\xi_g f_{gi}^{k+\frac{1}{2}} (a_{\alpha i} I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}} + b_{\alpha i} I_{\alpha i-\frac{1}{2}}^{k+\frac{1}{2}})}{(a_{\alpha i} I_{\alpha i+\frac{1}{2}}^{k+\frac{1}{2}} + b_{\alpha i} I_{\alpha i-\frac{1}{2}}^{k+\frac{1}{2}})} \right]$$
$$= \sum_g \frac{1}{\hat{\sigma}_{gi}} (I_{\alpha gi+\frac{1}{2}}^{k+\frac{1}{2}} - I_{\alpha gi-\frac{1}{2}}^{k+\frac{1}{2}}) + \sum_g \xi_g f_{gi}^{k+\frac{1}{2}}$$

(A.5.11)

Here we have used (A.5.01) and (A.5.05).

Now it is trivial to see how all terms except S_{gi} on the right hand side of (A.5.06) cancel each other.

A.6 BOUNDARY CONDITIONS OF THE DIFFUSION EQUATION:

The boundary conditions[A/2] are obtained by adding a term into the flux (scalar intensity) at cell boundaries in order to make it consistent with the scalar intensity inside the slab. Conventionally, a quantity known as the one-way flux must be conserved between the accelerated and non-accelerated equations.

The one way flux at the left and right boundaries is given as,

$$J_{\frac{1}{2}}^{l+\frac{1}{2}} = \Sigma_{\mu_m>0}\ \omega_m \mu_m I_{mg\frac{1}{2}}^{l+\frac{1}{2}}$$
$$J_{I+\frac{1}{2}}^{l+\frac{1}{2}} = \Sigma_{\mu_m<0}\ \omega_m \mu_m I_{mgI+\frac{1}{2}}^{l+\frac{1}{2}}$$

(A.6.01)

The diffusion equation derived here is based on the fact that if the specific intensity is linear in angular space, then the exact solution of the diffusion equation is obtained without iteration (**assuming** no negative flux fixup is implemented). The specific intensity at the boundaries is defined as

$$I_{mg}^{l+\frac{1}{2}} = \frac{1}{2} I_{0g}^{l+\frac{1}{2}} + \frac{3}{2}\mu_m I_{1g}^{l+\frac{1}{2}}$$

(A.6.02)

The one way flux becomes

$$J_{\frac{1}{2}}^{l+\frac{1}{2}} = \Sigma_{\mu_m>0}\ \omega_m \mu_m [\frac{1}{2} I_{0g\frac{1}{2}}^{l+\frac{1}{2}} + \frac{3}{2}\mu_m I_{1g\frac{1}{2}}^{l+\frac{1}{2}}]$$
$$J_{I+\frac{1}{2}}^{l+\frac{1}{2}} = \Sigma_{\mu_m<0}\ \omega_m \mu_m [\frac{1}{2} I_{0gI+\frac{1}{2}}^{l+\frac{1}{2}} + \frac{3}{2}\mu_m I_{1gI+\frac{1}{2}}^{l+\frac{1}{2}}]$$

(A.6.03a,b)

It's accelerated form is given as

$$J^{l+1}_{\frac{1}{2}} = \Sigma_{\mu_m>0}\ \omega_m\mu_m[\frac{1}{2}I^{l+1}_{0g\frac{1}{2}} + \frac{3}{2}\mu_m I^{l+1}_{1g\frac{1}{2}}]$$
$$J^{l+1}_{I+\frac{1}{2}} = \Sigma_{\mu_m<0}\ \omega_m\mu_m[\frac{1}{2}I^{l+1}_{0gI+\frac{1}{2}} + \frac{3}{2}\mu_m I^{l+1}_{1gI+\frac{1}{2}}]$$

(A.6.04a,b)

By subtracting (A.6.03) from (A.6.04), and using the condition that $J^{l+1/2} = J^{l+1}$, we obtain the following accelerated diffusion intensity at the boundaries after summing over all angles

$$I^{l+1}_{0g\frac{1}{2}}\Sigma_{\mu_m>0}\ \omega_m\mu_m = I^{l+\frac{1}{2}}_{0g\frac{1}{2}}\Sigma_{\mu_m>0}\ \omega_m\ \mu_m + I^{l+\frac{1}{2}}_{1g\frac{1}{2}} - I^{l+1}_{1g\frac{1}{2}}$$
$$I^{l+1}_{0gI+\frac{1}{2}}\Sigma_{\mu_m<0}\omega_m\mu_m = I^{l+\frac{1}{2}}_{0gI+\frac{1}{2}}\Sigma_{\mu_m<0}\ \omega_m\mu_m + I^{l+\frac{1}{2}}_{1gI+\frac{1}{2}} - I^{l+1}_{1gI+\frac{1}{2}}$$
$$\textit{since}\quad \Sigma_m\ \omega_m\mu_m^2 = \frac{1}{3}$$

(A.6.05a,b)

However $I^{l+1}{}_{1g1/2}$ and $I^{l+1}{}_{1gI+1/2}$ are unknown. To find expressions for these variables in terms of $I^{l+1}{}_{0gi\pm1/2}$ quantities we go back to the original equation used to derive the diffusion equation within the slab.

$I^{l+1}{}_{1g1/2}$ and $I^{l+1}{}_{1gI+1/2}$ are computed as follows

A. $I^{l+1}{}_{1g1/2}$

i. Divide (A.4.06) by σ_{gi}

ii. Substitute (A.4.07) in above for n=1

iii. Multiply (A.4.05) by (-1/2) and add the resultant into above

iv. Substitute (A.4.06) for n=0 into iv

v. Solve for $I^{l+1}{}_{1g1/2}$ by taking i = 1

B. $I^{l+1}{}_{1gI+1/2}$

A similar procedure is used, except that we now multiply by 1/2 (instead of -1/2) and solve for $I^{k-1}{}_{1gI+1/2}$ by taking i = I (instead of i=1), The final result is

$$I^{l+1}_{1g\frac{1}{2}} = \frac{\hat{\sigma}_{gl}}{4}(a_{0gl}I^{l+1}_{0g\frac{3}{2}} + b_{0gl}I^{l+1}_{0g\frac{1}{2}}) - \frac{\chi_{gl}\eta_1\Delta x_1}{4}\Sigma_g\ \sigma_{gl}(a_{0gl}I^{l+1}_{0g\frac{3}{2}} + b_{0gl}I^{l+1}_{0g\frac{1}{2}})$$
$$-\frac{\Delta x_1 Q_{0gl}}{2} + \frac{Q_{1gl}\Delta x_1}{\hat{\sigma}_{gl}} - \frac{1}{3\hat{\sigma}_{gl}}(I^{l+1}_{0g\frac{3}{2}} - I^{l+1}_{0g\frac{1}{2}}) - \frac{2}{3\hat{\sigma}_{gl}}(I^{l+\frac{1}{2}}_{2g\frac{3}{2}} - I^{l+\frac{1}{2}}_{2g\frac{1}{2}})$$

$$I^{l+1}_{1gl+\frac{1}{2}} = -\frac{\hat{\sigma}_{gl}}{4}(a_{0gl}I^{l+1}_{0gl+\frac{1}{2}} + b_{0gl}I^{l+1}_{0gl-\frac{1}{2}}) + \frac{\chi_{gl}\eta_l\Delta x_l}{4}\Sigma_g\ \sigma_{gl}(a_{0gl}I^{l+1}_{0gl+\frac{1}{2}} + b_{0gl}I^{l+1}_{0gl-\frac{1}{2}})$$
$$+\frac{\Delta x_l Q_{0gl}}{2} + \frac{Q_{1gl}\Delta x_l}{\hat{\sigma}_{gl}} - \frac{1}{3\sigma_{gl}}(I^{l+1}_{0gl+\frac{1}{2}} - I^{l+1}_{0gl-\frac{1}{2}}) - \frac{2}{3\hat{\sigma}_{gl}}(I^{l+\frac{1}{2}}_{2gl+\frac{1}{2}} - I^{l+\frac{1}{2}}_{2gl-\frac{1}{2}})$$

(A.6.06a,b)

After substituting (A.6.06) in (A.6.05), we rewrite these equations in similar form as the diffusion equation. The final form of the accelerated diffusion equation at the boundaries is given as

$$(\Sigma_{\mu_m>0}\ \omega_m\mu_m + \frac{\hat{\sigma}_{gl}}{4}b_{0gl} + \frac{1}{3\hat{\sigma}_{gl}})I^{l+1}_{0g\frac{1}{2}} + (\frac{\hat{\sigma}_{gl}}{4}a_{0gl} - \frac{1}{3\hat{\sigma}_{0gl}})I^{l+1}_{0g\frac{3}{2}}$$
$$= I^{l+\frac{1}{2}}_{0g\frac{1}{2}}\Sigma_{\mu_m>0}\ \omega_m\mu_m + I^{l+\frac{1}{2}}_{1g\frac{1}{2}} + \frac{\chi_{gl}\eta_1\Delta x_1}{4}\Sigma_g\ \sigma_{gl}(a_{0gl}I^{l+1}_{0g\frac{3}{2}} + b_{0gl}I^{l+1}_{0g\frac{1}{2}})$$
$$+\frac{\Delta x_1 Q_{0gl}}{2} - \frac{Q_{1gl}\Delta x_1}{\hat{\sigma}_{gl}} + \frac{2}{3\hat{\sigma}_{gl}}(I^{l+\frac{1}{2}}_{2g\frac{3}{2}} - I^{l+\frac{1}{2}}_{2g\frac{1}{2}})$$

$$(-\Sigma_{\mu_m<0}\ \omega_m\mu_m + \frac{\hat{\sigma}_{gl}}{4}a_{0gl} + \frac{1}{3\hat{\sigma}_{gl}})I^{l+1}_{0gl+\frac{1}{2}} + (\frac{\hat{\sigma}_{gl}}{4}b_{0gl} - \frac{1}{3\hat{\sigma}_{gl}})I^{l+1}_{0gl-\frac{1}{2}}$$
$$= -I^{l+\frac{1}{2}}_{0gl+\frac{1}{2}}\Sigma_{\mu_m<0}\omega_m\mu_m - I^{l+\frac{1}{2}}_{1gl+\frac{1}{2}} + \frac{\chi_{gl}\eta_l\Delta x_l}{4}\Sigma_g\ \sigma_{gl}(a_{0gl}I^{l+1}_{0gl+\frac{1}{2}} + b_{0gl}I^{l+1}_{0gl-\frac{1}{2}})$$
$$+\frac{\Delta x_l Q_{0gl}}{2} + \frac{Q_{1gl}\Delta x_l}{\hat{\sigma}_{gl}} - \frac{2}{3\hat{\sigma}_{gl}}I_{0g}(I^{l+\frac{1}{2}}_{2gl+\frac{1}{2}} - I^{l+\frac{1}{2}}_{2gl-\frac{1}{2}})$$

(A.6.07a,b)

A.7 BOUNDARY CONDITIONS OF THE GREY EQUATION:

The boundary conditions for the grey equation are obtained from the diffusion boundary conditions using the transformation (A.5.02) that was used to obtain the grey equation from the diffusion equation inside the slab. The following steps are used:

i. Substitute (A.5.01) in (A.6.06).

ii. Sum over frequency groups.

iii. Use similar simplification as was done to obtain (A.5.06) from (A.5.04).

The final form of the grey equation at the boundaries can then be expressed as

$$\begin{aligned}
&\Big(\Sigma_{\mu_m>0}\,\omega_m\mu_m + \Sigma_g\frac{\varphi_{gl}}{3\hat{\sigma}_{gl}} + \frac{1}{4}\xi_1 b_{01}\Big)I_{0\frac{1}{2}}^{k+1} + \Big(\frac{1}{4}\xi_1 a_{01} - \Sigma_g\frac{1}{3\hat{\sigma}_{gl}}\varphi_{gl}\Big)I_{0\frac{3}{2}}^{k+1} \\
&= I_{0\frac{1}{2}}^{l+\frac{1}{2}}\Sigma_{\mu_m>0}\omega_m\mu_m + I_{1\frac{1}{2}}^{l+\frac{1}{2}} - \frac{1}{4}\Sigma_g\xi_{gl}f_{gl}^{k+\frac{1}{2}} + \frac{\xi_1}{4}\Big(a_{01}I_{0\frac{3}{2}}^{k+\frac{1}{2}} + b_{01}I_{0\frac{1}{2}}^{k+\frac{1}{2}}\Big) \\
&\quad + \frac{\Delta x_1}{2}\Sigma_g Q_{0gl} - \Sigma_g\frac{Q_{1gl}\Delta x_1}{\hat{\sigma}_{gl}} + \Sigma_g\frac{2}{3\hat{\sigma}_{gl}}\Big(I_{2g\frac{3}{2}}^{l+\frac{1}{2}} - I_{2g\frac{1}{2}}^{l+\frac{1}{2}}\Big) \\
&\quad - \frac{1}{3}\Sigma\frac{\varphi_{gl}^{k+\frac{1}{2}}}{\hat{\sigma}_{gl}}\Big(I_{0\frac{3}{2}}^{k+\frac{1}{2}} - I_{0\frac{1}{2}}^{k+\frac{1}{2}}\Big) + \frac{1}{3}\Sigma\Big(\frac{1}{\hat{\sigma}_{gl}}\Big(I_{0g\frac{3}{2}}^{k+\frac{1}{2}} - I_{0g\frac{1}{2}}^{k+\frac{1}{2}}\Big)
\end{aligned}$$

(A.7.01;02)

A.8 SOLUTION OF THE DIFFUSION AND GREY EQUATIONS:

To obtain the solution for the diffusion equation, we rewrite (A.4.08) and (A.6.07) in a tridiagonal form, and invert the matrix. In matrix form (A.4.08) is written as

$$a_{gi}I_{0gi-\frac{1}{2}}^{l+1} + b_{gi}I_{0gi+\frac{1}{2}}^{l+1} + c_{gi}I_{0gi+\frac{3}{2}}^{l+1} = R_{gi}^{l+1}$$

(A.8.01)

where coefficients from (A.4.08) for i=2..I are given as

$$a_{gi} = -\frac{1}{3\hat{\sigma}_{gi-1}} + \frac{\hat{\sigma}_{gi-1}}{4} b_{0gi-1}$$

$$b_{gi} = \frac{1}{3\hat{\sigma}_{gi}} + \frac{1}{3\hat{\sigma}_{gi-1}} + \frac{\hat{\sigma}_{gi} b_{0gi}}{4} + \frac{\hat{\sigma}_{gi-1} a_{0gi-1}}{4}$$

$$c_{gi} = -\frac{1}{3\hat{\sigma}_{gi}} + \frac{\hat{\sigma}_{gi} a_{0gi}}{4}$$

$$R_{gi}^{l+1} = \frac{1}{4}\Sigma_l^* \left[\chi_{gi-1}\eta_{i-1}\Delta x_{i-1}\Sigma_g \sigma_{gi-1}(a_{0gi-1} I_{0gi-\frac{1}{2}}^{l+1} + b_{0gi} I_{gi-\frac{3}{2}}^{l+1})\right] + S_{gi-1}^{l+\frac{1}{2}}$$

(A.8.02a,b,c,d)

The expression for left and right boundaries from (A.6.07) are

$$a_{g1} = 0.0$$

$$b_{g1} = \Sigma_{\mu_m>0}\omega_m\mu_m + \frac{1}{3\hat{\sigma}_{g1}} + \frac{1}{4}\hat{\sigma}_{g1} b_{0g1}$$

$$c_{g1} = -\frac{1}{3\hat{\sigma}_{g1}} + \frac{1}{4}\hat{\sigma}_{g1} a_{0g1}$$

$$R_{g1}^{l} = I_{0g\frac{1}{2}}^{l+\frac{1}{2}}\Sigma_{\mu_m>0}\omega_m\mu_m + I_{1g\frac{1}{2}}^{l+\frac{1}{2}} + \frac{\Delta x_1 Q_{0g1}}{2} - \frac{\Delta x_1 Q_{1g1}}{\hat{\sigma}_{g1}}$$

$$+\frac{2}{3\hat{\sigma}_{g1}}(I_{2g\frac{3}{2}}^{l+\frac{1}{2}} - I_{2g\frac{1}{2}}^{l+\frac{1}{2}}) + \frac{1}{4}\chi_{g1}\eta_1\Delta x_1\Sigma_g \sigma_{g1}(a_{0g1} I_{0g\frac{3}{2}}^{l+1} + b_{0g1} I_{0g\frac{1}{2}}^{l+1})$$

(A.8.03a,b,c,d)

$$a_{gi+1} = \frac{1}{4}\hat{\sigma}_{gi} b_{0gi-1} - \frac{1}{3\hat{\sigma}_{gi-1}}$$

$$b_{gi+1} = -\Sigma_{\mu_m<0}\omega_m\mu_m + \frac{1}{3\hat{\sigma}_{gi-1}} + \frac{1}{4}\hat{\sigma}_{gi-1} a_{0gi-1}$$

$$c_{gi+1} = 0.0$$

$$R_{gi+1} = -I_{0gi+\frac{1}{2}}^{l+\frac{1}{2}}\Sigma_{\mu_m<0}\omega_m\mu_m - I_{1gi+\frac{1}{2}}^{l+\frac{1}{2}} + \frac{\Delta x_i Q_{0gi}}{2} + \frac{\Delta x_i Q_{1gi}}{\hat{\sigma}_{gi}}$$

$$-\frac{2}{3\hat{\sigma}_{gi}}(I_{2gi+\frac{1}{2}}^{l+\frac{1}{2}} - I_{2gi-\frac{1}{2}}^{l+\frac{1}{2}}) + \frac{1}{4}\chi_{gi}\eta_i\Delta x_i\Sigma_g \sigma_{gi}(a_{0gi} I_{0gi+\frac{1}{2}}^{l+1} + b_{0gi} I_{gi-\frac{1}{2}}^{l+1})$$

(A.8.04a,b,c,d)

In the source iteration method a new solution is substituted in (A.8.02d;3d) and the matrix is inverted again for the new solution. This is repeated until some desired convergence is achieved. To accelerate the diffusion equation we solve the

grey equation instead of substituting the new solution on the right side of the diffusion equation. The Grey equation is solved in like manner to the diffusion equation. The set of equations is given as

$$a_i I_{\alpha-\frac{1}{2}}^{k+\frac{1}{2}} + b_i I_{\alpha+\frac{1}{2}}^{k+\frac{1}{2}} + c_i I_{\alpha+\frac{3}{2}}^{k+\frac{1}{2}} = R_i^k$$

(A.8.05)

where coefficients from (A.5.04) for i=2..N are given as,

$$a_i = -\frac{1}{3}\Sigma_g \frac{\varphi_{gi-1}}{\hat{o}_{gi-1}} + \frac{1}{4}\xi_{i-1} b_{\alpha-1}$$

$$b_i = \frac{1}{3}\Sigma_g \left[\frac{\varphi_{gi}}{\hat{o}_{gi}} + \frac{\varphi_{gi-1}}{\hat{o}_{gi-1}}\right] + \frac{1}{4}\left[\xi_i b_\alpha + \xi_{i-1} a_{\alpha-1}\right]$$

$$c_i = -\frac{1}{3}\Sigma_g \frac{\varphi_{gi}}{\hat{o}_{gi}} + \frac{1}{4}\xi_i a_\alpha$$

For linear case

$$R_i^{k+\frac{1}{2}} = \Sigma_g \frac{1}{3\hat{o}_{gi+1}}\left(I_{\alpha gi+\frac{3}{2}}^{k+\frac{1}{2}} - I_{\alpha gi+\frac{1}{2}}^{k+\frac{1}{2}}\right) - \Sigma_g \frac{1}{3\hat{o}gi}\left(I_{\alpha gi+\frac{1}{2}}^{k+\frac{1}{2}} - I_{\alpha gi-\frac{1}{2}}^{k+\frac{1}{2}}\right)$$

$$- \frac{1}{3}\Sigma_g \frac{\varphi_{gi+1}}{\hat{o}_{gi+1}}\left(I_{\alpha+\frac{3}{2}}^{k+\frac{1}{2}} - I_{\alpha+\frac{1}{2}}^{k+\frac{1}{2}}\right) + \frac{1}{3}\Sigma_g \frac{\varphi_{gi}}{\hat{o}_{gi}}\left(I_{\alpha+\frac{1}{2}}^{k+\frac{1}{2}} - I_{\alpha-\frac{1}{2}}^{k+\frac{1}{2}}\right)$$

$$-\frac{1}{4}\Sigma_g\left[\xi_{gi+1} f_{gi+1}^{k+\frac{1}{2}} + \xi_{gi} f_{gi}^{k+\frac{1}{2}}\right] + \frac{1}{4}\xi_i\left[a_\alpha I_{\alpha+\frac{1}{2}}^{k+\frac{1}{2}} + b_\alpha I_{\alpha-\frac{1}{2}}^{k+\frac{1}{2}}\right]$$

$$+ \frac{1}{4}\xi_{i+1}\left[a_{\alpha+1} I_{\alpha+\frac{3}{2}}^{k+\frac{1}{2}} + b_{\alpha+1} I_{\alpha+\frac{1}{2}}^{k+\frac{1}{2}}\right] + \Sigma_g S_{gi}^{k+\frac{1}{2}}$$

For non linear case

$$R_i^{k+\frac{1}{2}} = \Sigma_g S_{gi}^{k+\frac{1}{2}}$$

(A.8.06a,b,c,d)

At the left and right boundaries from (A.7.01;02) we have

$$a_1 = 0.0$$

$$b_1 = \frac{1}{3}\Sigma_g \frac{\varphi_{gl}}{\hat{\sigma}_{gl}} + \frac{1}{4}\xi_1 b_{01} + \Sigma_{\mu_m>0}\omega_m\mu_m$$

$$c_1 = -\frac{1}{3}\Sigma_g \frac{\varphi_{gl}}{\hat{\sigma}_{gl}} + \frac{1}{4}\xi_1 a_{01}$$

For linear case

$$R_1^k = I_{0\frac{1}{2}}^{l+\frac{1}{2}}\Sigma_{\mu_m>0}\omega_m\mu_m + I_{1\frac{1}{2}}^{l+\frac{1}{2}} + \Sigma_g \frac{1}{3\hat{\sigma}_{gl}}(I_{0g\frac{3}{2}}^{k+\frac{1}{2}} - I_{0g\frac{1}{2}}^{k+\frac{1}{2}})$$

$$- \frac{1}{3}\Sigma_g \frac{\varphi_{gl}}{\hat{\sigma}_{gl}}(I_{0\frac{3}{2}}^{k+\frac{1}{2}} - I_{0\frac{1}{2}}^{k+\frac{1}{2}}) + \Sigma_g \frac{2}{3\hat{\sigma}_{gl}}(I_{2g\frac{3}{2}}^{l+\frac{1}{2}} - I_{2g\frac{1}{2}}^{l+\frac{1}{2}}) + \frac{\Delta x_1}{2}\Sigma Q_{0gl}$$

$$-\Delta x_1 \Sigma_g \frac{Q_{1gl}}{\hat{\sigma}_{gl}} - \frac{1}{4}\Sigma_g \xi_g f_{gl}^{k+\frac{1}{2}} + \frac{1}{4}\xi_1(a_{01}I_{0\frac{3}{2}}^{k+\frac{1}{2}} + b_{01}I_{0\frac{1}{2}}^{k+\frac{1}{2}})$$

For non linear case

$$R_1^k = I_{0\frac{1}{2}}^{l+\frac{1}{2}}\Sigma_{\mu_m>0}\omega_m\mu_m + I_{1\frac{1}{2}}^{l+\frac{1}{2}} + \Sigma_g \frac{2}{3\hat{\sigma}_{gl}}(I_{2g\frac{3}{2}}^{l+\frac{1}{2}} - I_{2g\frac{1}{2}}^{l+\frac{1}{2}})$$

$$+\frac{\Delta x_1}{2}\Sigma_g Q_{0gl} - \Delta x_1 \Sigma_g \frac{Q_{1gl}}{\hat{\sigma}_{gl}}$$

$$a_{I+1} = -\frac{1}{3}\Sigma_g \frac{\varphi_{gl}}{\hat{\sigma}_{gl}} + \frac{1}{4}\xi_I b_{0I}$$

$$b_{I+1} = \frac{1}{3}\Sigma_g \frac{\varphi_{gl}}{\hat{\sigma}_{gl}} + \frac{1}{4}\xi_I a_{0I} - \Sigma_{\mu_m<0}\omega_m\mu_m$$

$$c_{I+1} = 0.0$$

For linear case

$$R_{I+1}^{k+\frac{1}{2}} = -I_{0I+\frac{1}{2}}^{l+\frac{1}{2}}\Sigma_{\mu_m<0}\omega_m\mu_m - I_{1I\frac{1}{2}}^{l+\frac{1}{2}} - \Sigma_g \frac{1}{3\hat{\sigma}_{gl}}(I_{0gI+\frac{1}{2}}^{k+\frac{1}{2}} - I_{0gI-\frac{1}{2}}^{k+\frac{1}{2}})$$

$$+ \Sigma_g \frac{\varphi_{gl}}{3\hat{\sigma}_{gl}}(I_{0I+\frac{1}{2}}^{k+\frac{1}{2}} - I_{0I-\frac{1}{2}}^{k+\frac{1}{2}}) - \Sigma_g \frac{2}{3\hat{\sigma}_{gl}}(I_{2gI+\frac{1}{2}}^{l+\frac{1}{2}} - I_{2gI-\frac{1}{2}}^{l+\frac{1}{2}}) + \frac{\Delta x_I}{2}\Sigma Q_{0gl}$$

$$+\Delta x_I \Sigma_g \frac{Q_{1gl}}{\hat{\sigma}_{gl}} - \frac{1}{4}\Sigma_g \xi_g f_{gl}^{k+\frac{1}{2}} + \frac{1}{4}\xi_I(a_{0I}I_{0I+\frac{1}{2}}^{k+\frac{1}{2}} + b_{0I}I_{0I-\frac{1}{2}}^{k+\frac{1}{2}})$$

For non linear case

$$R_{I+1}^{k+\frac{1}{2}} = -I_{0I+\frac{1}{2}}^{l+\frac{1}{2}}\Sigma_{\mu_m<0}\omega_m\mu_m - I_{1I+\frac{1}{2}}^{l+\frac{1}{2}} - \Sigma_g \frac{2}{3\hat{\sigma}_{gl}}(I_{2gI+\frac{1}{2}}^{l+\frac{1}{2}} - I_{2gI-\frac{1}{2}}^{l+\frac{1}{2}})$$

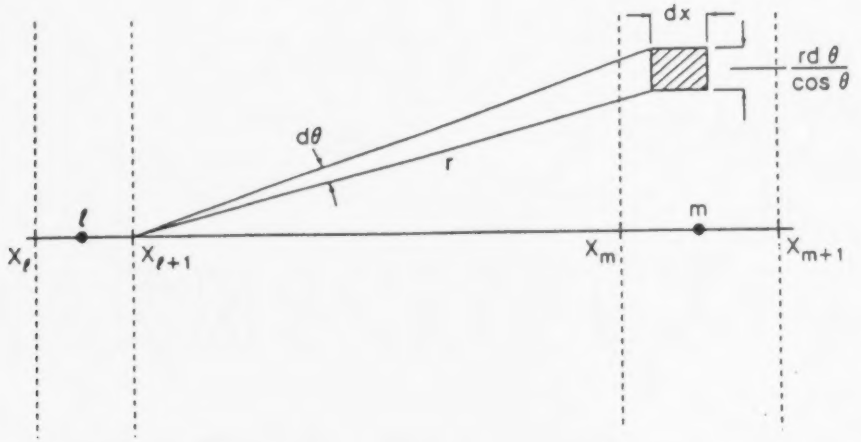
$$+\frac{\Delta x_I}{2}\Sigma_g Q_{0gl} + \Delta x_I \Sigma_g \frac{Q_{1gl}}{\hat{\sigma}_{gl}}$$

(A.8.07a,b,c;A.8.08a,b,c,d)

B. MARCHAND'S MODEL

Conceptually Marchand's approach is quite similar to the approach used by Audenaerde et al[B/1] to solve the neutron particle transport problem. The details of the mathematics involved can be found elsewhere[B/2]. The following discussion emphasises the conceptual understanding of Marchand's model in it's exact form and then the two-cell simplified model.

In order to elucidate Marchand's algorithm, consider the geometry shown in the figure below.



Using the analogy of the Andemaerde analysis, the radiation power intensity that originates from a ring of radius R of thickness dx in cell m and is incident on the right boundary of lth cell is

$$dP_{l+1}^{m}(\mu,\nu)d\mu d\nu = (2\pi RdRdx)d\nu\ n_m I_m \frac{\mu}{r^2} e^{-\tau(x_{l+1},x)/\mu} \qquad \text{(B.01)}$$

where $\mu = \cos\theta$ and τ is the optical depth between x_{l+1} and x, and can be expressed as

$$\tau(x_{l+1},x) = \tau(x_{l+1},x_m) + \tau(x_m,x) = \tau_{lm} + \frac{\tau(x-x_m)}{\Delta x_m}$$

(B.02)

where $\tau_m = n_m \sigma_m \Delta x_m$, n_m is the ion density, and I_m is the power radiated per atom, per unit frequency interval dν per unit solid angle in cell m.

The total radiation specific intensity from cell m incident on interface x_{l+1} is

$$P^m_{l+1}(\mu,\nu) = \int_0^{\Delta x_m} dP^m_{l+1}(\mu,\nu)dx$$

(B.03)

By using equation (B.01;02) in (B.03), (B.03) reduces to

$$P^m_{l+1}\, d\mu d\nu = \frac{2\pi I_m}{\sigma_m} \mu d\mu d\nu \; \{e^{-\frac{\tau_{lm}}{\mu}}\} \; \{1-e^{-\frac{\tau_m}{\mu}}\}$$

(B.04)

We can represent the contribution due to all cells left of cell l as

$$P^m_{l+1}\, d\mu = \sum_{m>l} \frac{2\pi I_m}{\sigma_m} \mu d\mu \; \{e^{-\frac{\tau_{lm}}{\mu}}\} \{1-e^{-\frac{\tau_m}{\mu}}\}$$

(B.05)

To compute the total intensity reaching position x_{l+1}(the right side of the cell) from all directions, we integrate over μ

$$Q^R_{l+1} = \int_0^1 d\mu P^R_{l+1}$$

$$Q^R_{l+1} = \sum_{m>l} \frac{2\pi I_m}{\sigma_m} \mu [E_3(\tau_{l,m}) - E_3(\tau_{l,m}+\tau_m)]$$

where $\qquad E_3(\tau) = \int_1^\infty \frac{dz}{z^3} e^{-\tau z}$

(B.06)

where E_3 is the exponential integral of order three. Similarly, the contribution from all directions at the left boundary of the cell is

$$Q_{l+1}^{L}=\sum_{m\le l}\frac{2\pi I_m}{\sigma_m}\mu[E_3(\tau_{l+1,m})-E_3(\tau_{l+1,m}+\tau_m)]$$

(B.07)

Then using the fact that energy is conserved, the net gain/loss of energy per unit volume and per unit energy in lth cell is

$$W_l=\frac{[Q_{l+1}^{R}-Q_l^{R}+Q_l^{L}-Q_{l+1}^{L}]}{\Delta x}$$

$$W_l=-\{\frac{4\pi I_l}{\Delta x\sigma_l}[\frac{1}{2}-E_3(\tau_l)]\}+\sum_{m\neq l}\frac{2\pi I_m}{\sigma_l\Delta x}\{E_3(\tau_{lm})-E_3(\tau_{lm}+\tau_l)$$
$$-E_3(\tau_{lm}+\tau_m)+E_3(\tau_{lm}+\tau_l+\tau_m)\}$$

(B.08)

Here the first term represents the power emitted out of cell l and the second term represents the power (emitted from all other cells and) absorbed by the lth cell. Unfortunately, due to coupling of each zone with other neighbouring zones, the simulation run times are significantly larger than those in which radiation is neglected.

In order to reduce the radiation time, Marchand developed an intuitive approach to solve the above problem. He claimed that one can approximate the plasma as being either optically thin or optically thick. In the limit where the plasma is optically thin, the intensity coming from the right (or left) of a given cell is the same as that produced by a single cell of luminosity equal to the sum of intensities emitted from all cells (since nothing is absorbed), that is

$$P_{l+1}=2\pi Z \qquad \textit{where} \qquad Z=\Sigma_m I_m\Delta x_m$$

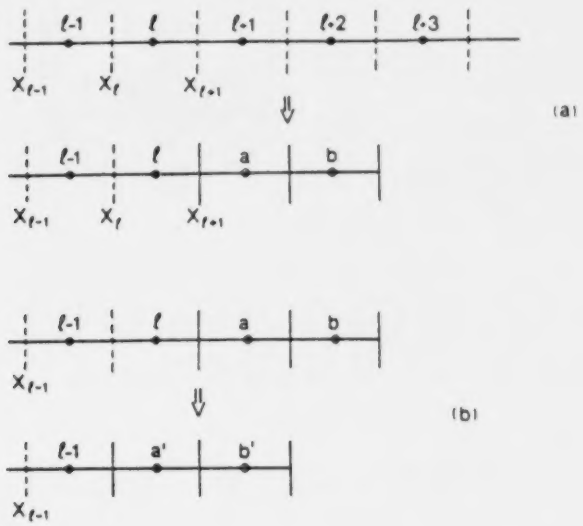
(B.09)

For the optically thick case, one treats it as if it is comprised of two cells, one optically thick (emission is negligible) and the other optically thin (here absorption is negligible), then the intensity emitted out of the original cell is

$$P(\mu)=2\pi Z_b e^{-\frac{\tau_a}{\mu}} \qquad \text{where} \qquad Z_b=I_b\Delta x_b$$

(B.10)

where cell "a" is non-radiating with optical thickness τ_a and cell "b" is optically thin and radiates with luminosity Z_b. Marchand called this approach of reducing n cells into two effective cells the **recursive approach**. The figure below illustrate what is meant by recursive approach.



In the recursive approach one assumes that the radiation intensity everywhere in the plasma can be approximated by the intensity generated by a combination of two cells, one optically thick and one optically thin. Following the preceding analysis, the intensity incident on the right boundary of the lth cell from the right is

$$P_l^R=2\pi Z_b e^{-\frac{\tau_b}{\mu}}=2\pi\mu\frac{I_l}{\sigma_l}(1-e^{-\frac{\tau_l}{\mu}})+Z_b e^{-\frac{(\tau_a+\tau_l)}{\mu}}$$

(B.11)

here the unknowns $Z_{b'}$ and $\tau_{a'}$ are chosen so that the dominant angular dependence

of the specific intensity is around $|\mu| = 1$; because in the cold region the specific intensity is strongly peaked around $|\mu| = 1$. With this simplification the number of computational operations is proportional to the number of cells N rather than N^2 as it is for the exact model.

To physically justify the applicability of his algorithm Marchand made some assumptions[B/3]. He assumed that for problems in consideration, the time scale which characterizes macroscopic changes of the medium is long compared to the typical photon transit time; hence to a good approximation radiation transport can be considered as a stationary problem. The range of energies is restricted to 30 ev < hν < 10 Kev for which photon scattering mean free paths are typically much longer than the absorption mean free path, implying scattering is negligible. In this limit, it is possible to describe the radiation transport in terms of photons being produced isotropically and propagating in straight lines until they are absorbed. The absorption probability is prescribed by the local absorption cross-section. Therefore, Marchand's model is applicable for problems in which time dependence or scattering can be ignored. The angular dependence of the intensity is ignored. Although our present radiation transport code also ignores scattering, the technique that is used to solve the radiative transfer equation can be made applicable ,with appropriate modification, to problems involving scattering.

C. LEE'S RADIATIVE TABLES

Spectral-line intensities from laser produced plasmas are useful as temperature and density diagnostics. These emission spectra allow one to test the accuracy of the theoretical rate coefficients. However, before one can predict the emission spectra, one needs to know the plasma's charge state distribution and ion-level population as a function of it's electron temperature and density.

The tables of emission spectra used in MEDUSA are produced by Y.T. Lee et al at Lawrence Livermore National Laboratory. A detailed description of the model used for Lee's table can be found elsewhere[C/1]. Here the formulation and regions of validity of these tables is briefly discussed.

Since the laser produced plasmas of interest are produced with electron density ranging from 10^{17} to 10^{21} cm^{-3}, neither the coronal nor the Saha-Boltzmann equilibrium models are applicable. The coronal model gives ionization balance for ions in their ground states, hence it's valid for plasmas with electron densities less than 10^{16} cm^{-3}. On the other hand, Saha-Boltzmann equation is only valid for higher density plasmas. The coronal model assumes that all ions in the plasma are in their ground state. The local thermodynamic equilibrium (LTE) model significantly over estimates the average ionization state at all temperature and the coronal model underestimates the ionization state at low temperature by neglecting excited sate ionization. Lee uses a kinetic model injunction with coronal and Saha-Boltzmann model to calculate the time dependent ionization balance and ion-level populations of the non-LTE plasma in the electron density range of interest. This model reduces to coronal equilibrium at low density and Saha-Boltzmann equilibrium at high density.

The ground-state and excited-state energy levels for each ionization stage are generated from screening constant calculated by W. Lokke et al and R. More. There is one energy level per principal quantum number, and quantum lowering is obtained from a modified Stewart and Pyatt formula to account for dense plasma effects. The following atomic process are included in the model

i. excitation and de-excitation collisions

ii. Radiative spontaneous emission

iii. Ionization due to collision

iv. Radiative recombination

v. Three body recombination

vi. Dielectronic recombination

The model assumes that each energy level couples with every level of the same ionization stage, but only to the ground state of the next ionization stage. The contribution of electron-impact ionization from excited levels is also taken into account.

The results of ionization balance model are used to normalized the relative populations that are determined by the balance of collisions and spontaneous radiative transitions to calculate spectral line intensity (of L shell transition) as a function of electron temperature and density. In the calculation, it is assumed that the effects of ionization and radiative recombination on the excited-state population are negligible, since electron collision rates are very large (of the order of 2) compare to both the ionization and radiative recombination rates at the temperatures and densities under consideration.

The model assumes that the plasma has small temperature and density gradients, and the effect of radiation transport is neglected. In situations where radiation transport and gradients are not negligible, the model is still useful in setting an upper bound for experimental data.

```
C2345678101234567820123456783012345678401234567850123456786012345678701234
C  ************************************************************************
C  *      RADIATIVE TRANSPORT CODE BY HUMAYON BUTT SEPT 92        *
C  *  TECHNIQUE USED IS CALLED DIFFUSION SYNTHETIC ACCELERATION   *
C  *          SEE M.Sc THESIS FOR DETAILS                         *
C  * DOCUMENTATION IS SHOWN IN LOWER CASE BUT ALL VARIABLES ARE   *
C  * MEANT TO BE IN UPPER CASE, f.e. (FOR EXAMPLE) IF YOU WANT TO *
C  * SCAN FOR "nrun" SCAN "NRUN"                                  *
C  ************************************************************************
C
      SUBROUTINE SATE

      PARAMETER (NANO=24,NFO=64,NCL=151)
      PARAMETER (RK=7.56066TE-16,PK=6.6261E-34)
      PARAMETER (BK=1.3807E-23,SP=3.0E08,EVE=1.6022E-19)
      PARAMETER (TCF=EVE/BK,PI=3.141593,A0=PK/(BK*TCF))

      INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      INTEGER DRT, DIFBC, DIFACC, IIT, TITA
      INTEGER INSB, IRUN, LIN, MEDUSA
      INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      INTEGER NRN, NCODE, NCOUNT, PRNT
      INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      INTEGER USC, WFN, CONV, DBXL, DBXU, NUM
      INTEGER NCP1, NCM1, NAD2
      INTEGER SMTST1, SMTST2, SMTST3, SMTST4, SMTST5
      INTEGER IT
      INTEGER MDT, NITT

      COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      COMMON /I2/ DRT, DIFBC, DIFACC, IIT, TITA
      COMMON /I3/ INSB, IRUN, LIN, MEDUSA
      COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      COMMON /I7/ USC, WFN, CONV, DBXL, DBXU, NUM
      COMMON /I8/ NCP1, NCM1, NAD2
      COMMON /SMT/ SMTST1, SMTST2, SMTST3, SMTST4, SMTST5
      COMMON /IMD/ MDT, NITT, RTEON

      REAL*8 ALFA(NCL), AC, ATMASS, DAF(NFG,NCL), ATEM(NCL)
      REAL*8 ABC(NFG,NCL), AB(NCL), AO(NFG,NCL)
      REAL*8 BETA(NCL), BO(NFG,NCL)
      REAL*8 CV(NCL), CW, CH(NFG,NCL)
      REAL*8 DL(NCL), DINT(NFG,NCL + 1), PRNTM
      REAL*8 DIST(NCL), DTIME, DSPR
      REAL*8 ETA(NCL)
      REAL*8 FINT(NFG,NCL + 1), FINL(NFG), FINR(NFG)
      REAL*8 FR(NFG + 1), FQ(NFG,NCL)
      REAL*8 HELIM
      REAL*8 INLB(NFG), INRB(NFG), ITSL, IERED(NCL), IERR
      REAL*8 INTB(NANG,NFG,NCL + 1), IINT(NANG,NFG,NCL), IZIN(NFG,NCL)
      REAL*8 ITRB, ITER(NFG,NCL)
      REAL*8 L, LFL, LOWLIM
      REAL*8 MAXT
      REAL*8 NATE(NCL), NINT(NANG,NFG,NCL)
      REAL*8 NFFT(NANG,NFG,NCL), NDIN(NFG,NCL + 1), NZIN(NFG,NCL)
      REAL*8 PMAC(NCL), PINT(NANG,NFG,NCL), PRTIME
      REAL*8 PGIN(NCL + 1), PFGI(NCL + 1), PLANK(NFG,NCL)
      REAL*8 PDIN(NFG,NCL + 1), PITE(NFG,NCL), PZIN(NFG,NCL)
      REAL*8 PAB(NCL)
      REAL*8 Q(NANG,NFG,NCL)
      REAL*8 SPH, SIRC, SPR
      REAL*8 SIGM(NFG,NCL), GRSI(NCL + 1)
      REAL*8 SOLU(NCL + 1), SPRB
      REAL*8 S(NFG,NCL), SUM1, SUM2, GRFQ(NCL), GRZQ(NCL)
      REAL*8 SINT(NFG,NCL + 1)
      REAL*8 TTIME, TOU, TERR, TELB
      REAL*8 TRNFVR(NCL), TEMP(NCL)
      REAL*8 UFL
      REAL*8 WP(NANG)
      REAL*8 ZLP(NANG), ZINT(NFG,NCL), ZQ(NFG,NCL), DIER

      COMMON /R01/ ALFA, AC, ATMASS, DAF, ATEM
      COMMON /R02/ ABC, AB, AO
      COMMON /R03/ BETA, BO
      COMMON /R04/ CV, CW, CH
      COMMON /R05/ DL, DINT, PRNTM
      COMMON /R06/ DIST, DTIME, DSPR
      COMMON /R07/ ETA
      COMMON /R071/ FINT, FINL, FINR
      COMMON /R08/ FR, FQ
      COMMON /R09/ HELIM
      COMMON /R10/ INLB, INRB, ITSL, IERED, IERR
      COMMON /R11/ INTB, IINT, IZIN
      COMMON /R12/ ITRB, ITER
      COMMON /R13/ L, LFL, LOWLIM
      COMMON /R14/ MAXT
      COMMON /R15/ NATE, NINT
      COMMON /R16/ NFFT, NDIN, NZIN
      COMMON /R17/ PMAC, PINT, PRTIME
      COMMON /R18/ PGIN, PFGI, PLANK
      COMMON /R181/ PDIN, PITE, PZIN
      COMMON /R182/ PAB
      COMMON /R19/ Q
      COMMON /R20/ SPH, SIRC, SPR
      COMMON /R21/ SIGM, GRSI
      COMMON /R22/ SOLU, SPRB
      COMMON /R23/ S, SUM1, SUM2, GRFQ, GRZQ
      COMMON /R231/ SINT
      COMMON /R24/ TTIME, TOU, TERR, TELB
      COMMON /R25/ TRNFVR, TEMP
      COMMON /R26/ UFL
      COMMON /R27/ WP
      COMMON /R28/ ZLP, ZINT, ZQ, DIER

C234567810123456782012345678301234567840123456785012345678601234567870123
      LOGICAL RTEON, TRN, DIFF, LOR, NLOR, SIMRUN, SMTST
      COMMON /L1/ TRN, DIFF, LOR, NLOR, SIMRUN, SMTST
      COMMON /RDC/ NRN, NCODE, NCOUNT, PRNT

C*** fsig & fsink are analytical expressions of sigma and
C   planckian function [eqn (4.2.09 & 4.2.07)]
      EXTERNAL FSIG, FPLNK, F2, F3

      IF (NCODE .EQ. 0) THEN
C**** ncode is set to 0 only once to read the input file "satein" when
C     this code is used to implement radiative effects in medusa, when
C     this code returns medusa ncode is set to 1.
C     "open" files related to this radiation code
C     "pcrdit" input data file for the radiation code
C     "analysis" error messages when this code becomes unstable
C     "inp" contains the temperature for the model problem
C     "result" contains values of the variables according to prm value
C**** parameter.
        OPEN (UNIT=4,FILE='satein',STATUS='OLD')
        OPEN (UNIT=99,FILE='analysis',STATUS='OLD')
        OPEN (UNIT=8,FILE='result',STATUS='OLD')
        OPEN (UNIT=7,FILE='inflow',STATUS='OLD')
        OPEN (UNIT=11,FILE='energy',STATUS='OLD')

C**** nrun=1 different runs with different time steps keeping everything
C     else same, only work for the model problem. Turned off for now.
        NRUN = 0
C**** scr=1 output if any to the files result, otherwise on the screen
C     num a debug varible - used to check consistency in IE & DSA
C     dbxl & dbxh used to print a variable(s) after dbxl # of iteration
C     until dbxh # of iterations, # of variable depends on the value of
C**** pres. tcont=1 means no parameter iteration.
        WRITE (6,*)'enter SCR NUM DBXL DBXU TCONT'
        READ (4,10) SCR, NUM, DBXL, DBXU, TCONT
   10   FORMAT (50X, I2, 1X, I2, 1X, I4, 1X, I4, 1X, I2)
        READ (4,20) SIMRUN
   20   FORMAT (66X, L2)
        WRITE (8,30) SCR, NUM, DBXL, DBXU, TCONT
   30   FORMAT (1X, 'SRC NUM DBXL DBXU TCONT =', 5(1X,I4))
        WRITE (8,40) SIMRUN
   40   FORMAT (1X, L2)
        IF (SCR .NE. 0) THEN
C**** place output in "satout" instead of on the screen
          OPEN (UNIT=6,FILE='satout',STATUS='OLD')
        END IF
C**** read initial data for the radiation code
C*********************************
        CALL DATAIN
C*********************************
C??     PRNT = PRES
        NCP1 = NC + 1
        NCM1 = NC - 1
        NAD2 = NA / 2
        SMTST = .FALSE.
        PRNTM = 1.00E-12
C**** read legendre polynomials's zeros and weight function
C*********************************
        CALL LPL
C*********************************
C**** initialize the iteration counter
        NCNT = 0
        TIT = 0
        OIT = 0
        IIT = 0
        TOIT = 0
        TIIT = 0
        COUNT = 0
        DCOUNT = 0
        NDICNT = 0
      END IF
      IT = 0
   50 TTIME = 0.0
      IF (SIMRUN) THEN
C**** this will simulate all possible combinations of si, dss without
C     grey and with (linear and nonlinear) grey with different bounds
C     (2,5,20,50,100,500) at different time steps (1,2,5,10,20,50,100,
C     200,500,1000) psec seconds. note this switch over rules any
C**** initial mode of acceleration.
        TRNACC = 0
        DIFACC = 0
        LIN = 0
        TRN = .FALSE.
        DIFF = .FALSE.
        LOR = .FALSE.
        NLOR = .FALSE.
C*********************************
        CALL RUNTST(IT)
C*********************************
C**** sets above simulation paprameters
      END IF
      CONT = 0
   60 CONTINUE
   70 IF (MEDUSA .EQ. 1) THEN
C**** get data necessary for medusa simulation
C     MDT acts as a switch to execute a part of tables subroutine
C     the subroutine reads the radiative tables and evaluates the
C     variables for the RTE, it's function is same as the model
C**** subroutine for the model problem.
        MDT = 0
C*********************************
        CALL TABLES
C*********************************
        MDT = 1
        IF (NITT .NE. 1 .OR. ( .NOT. RTEON)) RETURN
      ELSE
```

```
C***** define the model problem
C*********************************
      CALL MODEL
C*********************************
      END IF

C***** RT used as reset parameter for computation of spectral radius of
C     the transfer equation
C     smtst used to prevent the code from falling apart, these switches
C     stop further computation of an equation when it appears to be
C***** failing to converge or starts to diverge.
      RT = 0
   80 SMTST1 = 0
      SMTST2 = 0
      SMTST3 = 0
      SMTST4 = 0
      SMTST5 = 0

      TOIT = TOIT + 1
      IF (TOIT .GT. OITA) THEN
C***** compute new temperature
C*********************************
        CALL TEMPER
        CALL CPUTM
C*********************************
        WRITE (8,*)'program stoped because oita exceeded', TOIT, OITA
        STOP
      END IF
      IIT = 0
C***** DRT used as reset parameter for computation of spectral radius
C***** of the diffusion equation
      DRT = 0
C*********************************
C***** solve radiative transfer equation
      CALL TRNPRT
C*********************************
      OIT = OIT + 1
C***** check if radiative transfer equation is converged

      CALL TRCONV
C*********************************
      DO 110 J = 1, NO
        DO 100 K = 1, NC
          DO 90 I = 1, NA
            PINT(I,J,K) = NINT(I,J,K)
   90     CONTINUE
  100   CONTINUE
  110 CONTINUE
      IF (CONV .EQ. 0 .OR. OIT .GE. TB .OR. (SMTST)) THEN
C***** transport intensity is converged or transport bound is exceeded or
C***** smtst is true
        IF (SMTST) THEN
          WRITE (99,*)'outer iteration terminated due to spr .gt. 1.00 t
     1o often'
          SMTST = .FALSE.
        END IF
        GO TO 290
      END IF
      IF (TRNACC .EQ. 0) THEN
C*********************************
        CALL TRNEI
C***** solve transfer equation using source iteration.
C*********************************
        GO TO 80
      ELSE IF (TRNACC .EQ. 1) THEN
        IIT = 0
  120   TIIT = TIIT + 1
        DCOUNT = DCOUNT + NDSCNT
        NDSCNT = 0
C***** solve multifrequency diffusion equation
C*********************************
        CALL MFDE
C*********************************
C***** check if multifrequency diffusion equation is converged
C*********************************
        CALL DFCONV
C*********************************
        IIT = IIT + 1
        IF (IIT .GE. DB .OR. CONV .EQ. 0 .OR. (SMTST)) THEN
C***** diffusion equation is converged or diffusion bound is exceeded or
C***** smtst is true
          IF (NUM .EQ. 1) THEN
C***** used to compare converged accelerated and unaccelerated diffusion
C     intensity, I.I. (flat in) the solution of diffusion equation with
C***** SI and with gray diffusion equation
            WRITE (8,*)'nat tilt oit iit tit', TOIT, TIIT, OIT, IIT,
     1        TIT
            WRITE (98,130) ((I,K,NDIN(I,K),K=1,NCP1),I=1,NO)
  130       FORMAT (3(1X,I2,1X,I2,1X,1PE10.3,1X))
            WRITE (*,*)'enter 1 to continue'
            READ (5,*) NUM
            IF (NUM .NE. 1) THEN
              STOP
            END IF
          END IF
          IF (SMTST) THEN
            SMTST = .FALSE.
            IF (SMTST2 .OR. NO*NC*0.05) THEN
              WRITE (99,*)'inner iteration terminated due to too often i
     1ll solution at'
              SMTST2 = 0
            ELSE IF (SMTST3 .OR. NO*NC*0.01) THEN
              WRITE (99,*)'inner iteration terminated due to dspr .gt. 0
     1.99 too often'
              SMTST3 = 0
            END IF

      WRITE (99,140) TOIT, TIIT, OIT, TIT
  140   FORMAT (1X, 'toit=', I8, 1X, 'tiit=', I4, 1X, 'oit=', I4,
     1    1X, 'tit=', I4)
        END IF
        NDZI = 0
        DO 170 J = 1, NO
          DO 160 K = 1, NC
            ZINT(J,K) = (AO(J,K)*NDIN(J,K + 1) + BO(J,K)*NDIN(J,K)) /
     1      2
            IF (ZINT(J,K) .LE. 0.0) THEN
              NDZI = NDZI + 1
              WRITE (99,150) J, K, ZINT(J,K), TOIT, TIT
  150         FORMAT (1X, 'zint from diff is neg. j k zint toit tit',
     1          2(I2,1X), 1PE10.3, 2(1X,I2))
            END IF
  160     CONTINUE
  170   CONTINUE
C*****  WRITE (8,*)'zint neg. from diff this often',ndzi
        DO 190 K = 1, NC
          AB(K) = 0.0
          DO 180 J = 1, NO
            AB(K) = AB(K) + ABC(J,K) * ZINT(J,K)
  180     CONTINUE
  190   CONTINUE
        IF (ABVL .EQ. 1) THEN
C***** take absolute value of converged ndin when it is negative
          DO 210 K = 1, NC
            DO 200 J = 1, NO
              IF (NDIN(J,K) .LE. 0.0) THEN
                NDIN(J,K) = ABS(NDIN(J,K))
              END IF
  200       CONTINUE
  210     CONTINUE
        END IF
        DO 230 K = 1, NC
          IF (AB(K) .LE. 0.0) THEN
            WRITE (99,220) K, AB(K), TOIT, TIIT, OIT, TIT
  220       FORMAT (1X, 'ab(k) from diff is neg. may cause instability
     1', I2, 1X, 1PE11.3, 4(1X,I8))
          END IF
  230   CONTINUE
        GO TO 80
      END IF
  240 IF (DIFACC .LE. 1) THEN
C*****   solve diffusion equation using source iteration
C*********************************
        CALL DIFFEI
C*********************************
      ELSE IF (DIFACC .EQ. 2) THEN
C***** solve diffusion equation using gray equation
C*********************************
        CALL GRDE
C*********************************
      END IF
      NEGID = 0
      DO 260 K = 1, NCP1
        DO 250 J = 1, NO
          IF (NDIN(J,K) .LE. 0) THEN
            NEGID = NEGID + 1
          END IF
  250   CONTINUE
  260 CONTINUE
C*****    write(8,*)'ndin neg this often',negid
      DO 280 J = 1, NO
        DO 270 K = 1, NCP1
          DIN(J,K) = NDIN(J,K)
  270   CONTINUE
  280 CONTINUE
      GO TO 120
    END IF
C*****   compute new temperature
  290 TIT = TIT + 1
    OIT = 0
    DO 320 K = 1, NC
      DO 310 J = 1, NO
        ZINT(J,K) = 0.0
        DO 300 I = 1, NA
          ZINT(J,K) = ZINT(J,K) + NINT(I,J,K) * WF(I)
  300   CONTINUE
  310 CONTINUE
  320 CONTINUE
    IF (NUM .EQ. 0) THEN
C*****    used to compare converged accelerated and unccelerated zint
C*****    I.I. solution of the RTE with SI and with diffusion equation
      WRITE (8,*)'j k zint', TOIT, TIIT, OIT, IIT, TIT
      WRITE (98,330) ((J,K,ZINT(J,K),K=1,NC),J=1,NO)
  330 FORMAT (3(1X,I2,1X,I2,1X,1PE10.3,1X))
C*********************************
      CALL CPUTM
C*********************************
      WRITE (*,*)'enter 0 to continue'
      READ (5,*) NUM
      IF (NUM .NE. 0) THEN
        STOP
      END IF
    END IF
    DO 350 K = 1, NC
      AB(K) = 0.0
      DO 340 J = 1, NO
        AB(K) = AB(K) + ABC(J,K) * ZINT(J,K)
  340 CONTINUE
  350 CONTINUE
    DO 370 K = 1, NC
      IF (AB(K) .LE. 0) THEN
        WRITE (8,360) K, TOIT, OIT, TIT, AB(K)
  360   FORMAT (1X, 'temp may become neg. k toit oit tit ab(k)',
```

```
      1        4(1X,I8), 1X, 11PE10.3)
         END IF
  370 CONTINUE
C****    WRITE (*,*)'test tit tit', TOIT, TIIT, TIT
      IF (MEDUSA .EQ. 0) THEN
C****    compute new temperature
C*********************************
         CALL TEMPER
C*********************************
C**** check if new temperature is converged
C*********************************
         CALL TEMCON
C*********************************
         IF (SIMRUN) THEN
          IF (CONT .EQ. 0) THEN
C*********************************
            CALL CPUTM
C*********************************
            CALL RUNTST(IT)
C*********************************
            GO TO 60
           ELSE
            GO TO 70
           END IF
          END IF
          IF (CONT .EQ. 0 .OR. TIT .GE. TITA) THEN
           IF (TIT .GE. TITA) THEN
            WRITE (8,380) TTIME
  380       FORMAT (1X, 'unconverged temperature at time:', 1PE11.4)
           ELSE
            WRITE (8,390) TTIME
  390       FORMAT (1X, 'converged temperature at time:', 1PE11.4)
           END IF
C*********************************
           CALL CPUTM
C*********************************
           IF (NRUN .EQ. 0) THEN
            STOP
           END IF
           NCNT = NCNT + 1
           IF (NCNT .EQ. 1) THEN
            DTIME = 1.00E-11
           ELSE IF (NCNT .EQ. 2) THEN
            DTIME = 1.00E-10
           ELSE IF (NCNT .EQ. 3) THEN
            DTIME = 2.00E-10
           ELSE IF (NCNT .EQ. 4) THEN
            DTIME = 4.00E-10
           ELSE IF (NCNT .EQ. 5) THEN
            DTIME = 6.00E-10
           ELSE IF (NCNT .EQ. 6) THEN
            DTIME = 1.00E-09
           ELSE IF (NCNT .EQ. 7) THEN
            DTIME = 1.60E-09
           ELSE IF (NCNT .EQ. 8) THEN
            DTIME = 2.00E-09
           ELSE IF (NCNT .EQ. 9) THEN
            DTIME = 3.00E-09
           ELSE IF (NCNT .EQ. 10) THEN
            DTIME = 5.00E-09
           ELSE IF (NCNT .EQ. 11) THEN
            DTIME = 1.00E-08
           ELSE IF (NCNT .EQ. 12) THEN
            DTIME = 1.00E-07
           ELSE
            STOP
           END IF
           TIT = 0
           OIT = 0
           IIT = 0
           TOIT = 0
           TIIT = 0
           COUNT = 0
           DCOUNT = 0
           NDICNT = 0
           GO TO 50
          ELSE
C**** solve the transfer equation again
           GO TO 70
          END IF
         ELSE
C*********************************
          CALL TABLES
C*********************************
         END IF
         END
C
C ***************************************************************************
C *    read the input                                                       *
C ***************************************************************************
C
         SUBROUTINE DATAIN

         PARAMETER (NANO=24,NFO=64,NCL=151)
         PARAMETER (BK=7.560667E-16,PK=6.6261E-34)
         PARAMETER (SK=1.3807E-23,SP=3.0E08,EVB=1.6022E-19)
         PARAMETER (TCF=EVE/BK,PI=3.141593,A0=PK/(BK*TCF))

         INTEGER SETLIM

         INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
         INTEGER DIRT, DIFBC, DIFACC, IIT, TITA
         INTEGER INSB, IRUN, LIN, MEDUSA
         INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
         INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
         INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
```

```
         INTEGER USC, WFN, CONV, DBXL, DBXU, NUM

         COMMON /1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
         COMMON /2/ DIRT, DIFBC, DIFACC, IIT, TITA
         COMMON /3/ INSB, IRUN, LIN, MEDUSA
         COMMON /4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
         COMMON /5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
         COMMON /6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
         COMMON /7/ USC, WFN, CONV, DBXL, DBXU, NUM

         REAL*8 ALFA(NCL), AC, ATMASS, DAF(NFO,NCL), ATEM(NCL)
         REAL*8 DIST(NCL), DTIME, DSPR
         REAL*8 HELIM
         REAL*8 INLB(NFO), INRB(NFO), ITSL, IERED(NCL), IERR
         REAL*8 INTB(NANO,NFO,NCL + 1), IINT(NANO,NFO,NCL), IZIN(NFO,NCL)
         REAL*8 ITRB, ITER(NFO,NCL)
         REAL*8 L, LFL, LOWLIM
         REAL*8 MAXT
         REAL*8 PMAC(NCL), PINT(NANO,NFO,NCL), PRTIME
         REAL*8 SPH, SERC, SPR
         REAL*8 SOLU(NCL + 1), SPRB
         REAL*8 TTIME, TOU, TERR, TELB
         REAL*8 UFL
         REAL*8 ZLP(NANO), ZINT(NFO,NCL), ZQ(NFO,NCL), DIER

         COMMON /R01/ ALFA, AC, ATMASS, DAF, ATEM
         COMMON /R06/ DIST, DTIME, DSPR
         COMMON /R09/ HELIM
         COMMON /R10/ INLB, INRB, ITSL, IERED, IERR
         COMMON /R11/ INTB, IINT, IZIN
         COMMON /R12/ ITRB, ITER
         COMMON /R13/ L, LFL, LOWLIM
         COMMON /R14/ MAXT
         COMMON /R17/ PMAC, PINT, PRTIME
         COMMON /R20/ SPH, SERC, SPR
         COMMON /R22/ SOLU, SPRB
         COMMON /R24/ TTIME, TOU, TERR, TELB
         COMMON /R26/ UFL
         COMMON /R28/ ZLP, ZINT, ZQ, DIER

         WRITE (6,*)'ENTER "0" IF SOUCRE IS TO BE DEPENDENT ON TIME'
         READ (4,10) TEMPTD
  10     FORMAT (66X, I2)
         WRITE (8,20) TEMPTD
  20     FORMAT (1X, 'TEMPTD = ', I2)
         WRITE (6,*)'ENTER "0" IF INITIAL TEMPERATURE DURIBUTION IS EXPON
        1ANTIAL'
         READ (4,30) TEMEXP
  30     FORMAT (66X, I2)
         WRITE (8,40) TEMEXP
  40     FORMAT (1X, 'TEMEXP = ', I2)
         READ (4,50) NFMUST
  50     FORMAT (66X, I2)
         WRITE (8,60) NFMUST
  60     FORMAT (1X, 'NFMUST = ', I2)
         WRITE (6,*)'ENTER "0 TO 20" FOR VARIABLE PRINTOUT'
         READ (4,70) PRES
  70     FORMAT (66X, I2)
         WRITE (8,80) PRES
  80     FORMAT (1X, 'PRES  = ', I2)
         WRITE (6,*)'ENTER BOUND FOR TRANSPORT AND DIFFUSION EQU'
         READ (4,90) TB, DB
  90     FORMAT (60X, I4, 1X, I3)
         WRITE (8,100) TB, DB
 100     FORMAT (1X, 'TB  DB = ', 1X, 2I5))
         WRITE (6,*)'ENTER "0"IF IN NFP INTENSITY AT CELL BOUNDARY IS TO
        1BE'
         WRITE (6,*)'ZERO OR "1" IF IT IS TO BE CELL AVERAGE INTENSITY OR
        1 '
         WRITE (6,*)'"2" IF MTS PAPER CRIETRION IS TO BE USED'
         READ (4,110) NFPC
 110     FORMAT (66X, I2)
         WRITE (8,120) NFPC
 120     FORMAT (1X, 'NFPC  = ', I2)
         WRITE (6,*)'ENTER IERR AND TERR AND DIER'
         READ (4,130) IERR, TERR, DIER
 130     FORMAT (41X, 3(1X,1PE8.2))
         WRITE (8,140) IERR, TERR, DIER
 140     FORMAT (1X, 'IERR  = ', 1PE10.3, 5X, 'TERR = ', 1PE10.3, 5X,
        1     'DIER = ', 1PE10.3)
         WRITE (6,*)'ENTER #OF OIT AFTER WHICH NEGATIVE FLUX IS ALWAYS US
        1ED'
         READ (4,150) INSB
 150     FORMAT (62X, I3)
         WRITE (8,160) INSB
 160     FORMAT (1X, 'INSB  = ', I3)
         WRITE (6,*)'ENTER ABSORPTION COEFICIENT 1E? (? = 6 TO 11)'
         READ (4,170) AC
 170     FORMAT (60X, 1PE8.2)
         WRITE (8,180) AC
 180     FORMAT (1X, 'AC = ', 1PE10.3)
         WRITE (6,*)'ENTER 0 IF NDIF IS TO BE USED FOR CONVERGENCE OR "1"
         WRITE (6,*)'IF (NINT-PINT) IS TO BE USED AND "2" IF IT IS TO BE
        1NORMALIZ'
         READ (4,190) CONVC
 190     FORMAT (66X, I2)
         WRITE (8,200) CONVC
 200     FORMAT (1X, 'CONVC  = ', I2)
         READ (4,210) TRIN
 210     FORMAT (66X, I2)
         WRITE (8,220) TRIN
 220     FORMAT (1X, 'TRIN  = ', I2)
         WRITE (6,*)'ENTER "0" IF UNIFORM SPATIAL DURIBUTION IS TO BE USED'

         READ (4,230) USC
 230     FORMAT (66X, I2)
```

```
      WRITE (8,240) USC
  240 FORMAT (1X, 'USC    = ', I2)
      READ (4,250) PRTIME
  250 FORMAT (60X, 1PE8.2)
      WRITE (8,260) PRTIME
  260 FORMAT (1X, 'PRTIME  = ', 1PE11.2)
      WRITE (6,*)'ENTER "0 TO 2" FOR DIFFUSION BC'
      READ (4,270) DIFBC
  270 FORMAT (66X, I2)
      WRITE (8,280) DIFBC
  280 FORMAT (1X, 'DIFBC  = ', I2)
      WRITE (6,*)'ENTER "0" IF NEW DIFFUSION INTENSITY IS NEGATIVE IT I
     1S'
      WRITE (6,*)'TAKEN TO BE ZERO"1" IF IT IS TAKEN TO BE THE PREVIOU
     1S'
      WRITE (6,*)'INTENSITY FOR THAT GROUP & CELL'
      READ (4,290) NDIT
  290 FORMAT (66X, I2)
      WRITE (8,300) NDIT
  300 FORMAT (1X, 'NDIT   = ', I2)
      WRITE (6,*)'ENTER MAXIMUM TIME FOR SIMULATION OF MODEL PROBLEM'
      READ (4,310) MAXT
  310 FORMAT (60X, 1PE8.2)
      WRITE (8,320) MAXT
  320 FORMAT (1X, 'MAXT   = ', 1PE11.2)
      WRITE (6,*)'ENTER NA < 24  NG < 64  NC < 151 '
      READ (4,330) NA, NG, NC
  330 FORMAT (57X, I3, 1X, I3, 1X, I3)
      WRITE (8,340) NA, NG, NC
  340 FORMAT (1X, 'NA = ', I3, 5X, 'NG = ', I3, 5X, 'NC = ', I3)
      WRITE (6,*)'ENTER  L   LFL   UFL    TELB   ITRB   ITBL'
      READ (4,350) L, LFL, UFL, TELB, ITRB, ITBL
  350 FORMAT (/4X, 6(1X,1PE8.2))
      WRITE (8,360)
  360 FORMAT (1X, 4X, 'L', 8X, 'LFL', 6X, 'UFL', 5X, 'TELB', 5X, 'ITRB',
     1    5X, 'ITBL')
      WRITE (8,370) L, LFL, UFL, TELB, ITRB, ITBL
  370 FORMAT (1X, 6(1X,1PE8.2))
      WRITE (6,*)'ENTER "0",IF PLANCKIAN IS TO BE USED AS A WEIGHT'
      WRITE (6,*)'FUNCTION OR "1" IF ROSSLAND FUNCTIONS IS TO BE USED'
      READ (4,380) WFN
  380 FORMAT (66X, I2)
      WRITE (8,390) WFN
  390 FORMAT (1X, 'WFN    = ', I2)
      WRITE (6,*)'ENTER SPECIFIC HEAT'
      READ (4,400) SPH
  400 FORMAT (60X, 1PE8.2)
      WRITE (8,410) SPH
  410 FORMAT (1X, 'SPECIFIC HEAT = ', 1PE10.3)
      WRITE (6,*)'ENTER DTIME'
      READ (4,420) DTIME
  420 FORMAT (60X, 1PE8.2)
      WRITE (8,430) DTIME
  430 FORMAT (1X, 'DTIME  = ', 1PE10.3)
      NF = 0
      WRITE (6,440) NF
  440 FORMAT (1X, 'NF     = ', I2)
      WRITE (6,*)'ENTER NUMBER OF TEMPERATURE ITERATIONS ALLOWED'
      READ (4,450) TITA
  450 FORMAT (/64X, I4)
      WRITE (8,460) TITA
  460 FORMAT (1X, 'TITA   = ', I4)
      WRITE (6,*)'ENTER NUMBER OF OUTER ITERATIONS ALLOWED'
      READ (4,470) OITA
  470 FORMAT (62X, I6)
      WRITE (8,480) OITA
  480 FORMAT (1X, 'OITA   = ', I6)
      READ (4,490) SETLIM
  490 FORMAT (66X, I2)
      WRITE (8,500) SETLIM
  500 FORMAT (1X, 'SETLIM = ', I2)
      SETSOU = 2
      WRITE (6,*)'ENTER 0 IF FLUX AT RIGHT BOUNDAR IS 0, 1 IF BOTH END S
     1'
      READ (4,510) SETSOU
  510 FORMAT (66X, I2)
      WRITE (8,520) SETSOU
  520 FORMAT (1X, 'SETSOU = ', I2)
      WRITE (6,*)'ENTER "1" FOR A & B TO BE 1 AT BOUNDARIES'
      READ (4,530) ABVL
  530 FORMAT (66X, I2)
      WRITE (8,540) ABVL
  540 FORMAT (1X, 'ABVL   = ', I2)
      WRITE (6,*)'ENTER "1" IF CODE TO BE RUN WITH MEDUSA'
      READ (4,550) MEDUSA
  550 FORMAT (66X, I2)
      WRITE (8,560) MEDUSA
  560 FORMAT (1X, 'MEDUSA = ', I2)
      WRITE (6,*)'ENTER 1 IF CRITERIAN IS AUTOMATICALLY DECIDED DEPENDIN
     1G ON THE SPR OF'
      WRITE (6,*)'TRANSPORT EQn, ALSO ENTER THE VALEU FOR SPR FOR AUTOMA
     1TIC ACCELERATION (<.5)'
      READ (4,570) AUTACL, SPRB
  570 FORMAT (56X, I2, 2X, 1PE8.2)
      WRITE (6,*)'ENTER "0" IF TRANSPORT EQUATION IS TO BE SOLVED BY SI'
      WRITE (6,*)'OR "1" IF BY DSA'
      READ (4,580) TRNACC
  580 FORMAT (66X, I2)
      WRITE (8,590) TRNACC
  590 FORMAT (1X, 'TRNACC = ', I2)
      WRITE (6,*)'ENTER"1"IF DIFFUSION EQUATION IS TO BE ACCELERATED'
      WRITE (6,*)'USING GREY METHOD'
      READ (4,600) DIFACC
  600 FORMAT (66X, I2)
      WRITE (8,610) DIFACC
  610 FORMAT (1X, 'DIFACC = ', I2)
```



```
  620 WRITE (6,*)'ENTER "0" FOR LINEAR GREY MODEL OR "1" FOR NONLINEAR G
     1REY MODEL'
      READ (4,630) LIN
  630 FORMAT (66X, I2)
      WRITE (8,640) LIN
  640 FORMAT (1X, 'LIN    = ', I2)
      IF (SETLIM .EQ. 0) THEN
       LOWLIM = 60.0
       HILIM = 70.0
      ELSE IF (SETLIM .EQ. 1) THEN
       LOWLIM = 90.0
       HILIM = 100.0
      ELSE IF (SETLIM .EQ. 2) THEN
       LOWLIM = 140.0
       HILIM = 150.0
      ELSE IF (SETLIM .EQ. 3) THEN
       LOWLIM = 190.0
       HILIM = 200.0
      ELSE IF (SETLIM .EQ. 4) THEN
       LOWLIM = 290.0
       HILIM = 300.0
      ELSE IF (SETLIM .EQ. 5) THEN
       LOWLIM = 250.0
       HILIM = 300.0
      ELSE IF (SETLIM .EQ. 6) THEN
       LOWLIM = 690.0
       HILIM = 700.0
      END IF
      WRITE (8,650) LOWLIM, HILIM
  650 FORMAT (1X, 'lowlim=', 1PE10.3, 1X, 'hilim=', 1PE10.3)
      RETURN
      END
C
C     ******************************************************************
C     * this subroutine defines the model problem used to test the     *
C     * code. another user can modify the model by changing the        *
C     * variables in this subroutine, any change in other subroutine   *
C     * will result in alteration of the method itself.                *
C     ******************************************************************
C
      SUBROUTINE MODEL

      PARAMETER (NANG=24,NFG=64,NCL=151)
      PARAMETER (BK=7.560667E-16,PK=6.6261E-34)
      PARAMETER (BK=1.380 7E-23,SP=5.0808,EVB=1.6022E-19)
      PARAMETER (TCF=EVB/BK,GK=4.3144,PI=3.141593,A0=PK/(BK*TCF))
      PARAMETER (A1=3.8171E+55)

      REAL*8 DIB, D, E
      REAL*8 FP(NFG + 1,NCL), ITLB
      REAL*8 LLFL, LFIN, LFR(NFG + 1), LITLB, LUFL
      REAL*8 RES2, RES3
      REAL*8 TRNFV

      INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      INTEGER DRT, DIFBC, DIFACC, IIT, TITA
      INTEGER INSD, IRUN, LIN, MEDUSA
      INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      INTEGER USC, WFN, CONV, DBXL, DBXU, NUM
      INTEGER NCP1, NCM1, NAD2
      INTEGER SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

      LOGICAL TRN, DIFF, LOR, NLOR, SIMRUN, SMTST
      COMMON /L1/ TRN, DIFF, LOR, NLOR, SIMRUN, SMTST

      COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      COMMON /I2/ DRT, DIFBC, DIFACC, IIT, TITA
      COMMON /I3/ INSD, IRUN, LIN, MEDUSA
      COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      COMMON /I7/ USC, WFN, CONV, DBXL, DBXU, NUM
      COMMON /I8/ NCP1, NCM1, NAD2
      COMMON /SMT/ SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

      REAL*8 ALFA(NCL), AC, ATMASS, DAF(NFG,NCL), ATEM(NCL)
      REAL*8 ABC(NFG,NCL), AB(NCL), AO(NFG,NCL)
      REAL*8 BETA(NCL), BO(NFG,NCL)
      REAL*8 CV(NCL), CW, CH(NFG,NCL)
      REAL*8 DL(NCL), DINT(NFG,NCL + 1), PRNTM
      REAL*8 DIST(NCL), DTIME, DSPR
      REAL*8 ETA(NCL)
      REAL*8 FR(NFG + 1), FQ(NFG,NCL)
      REAL*8 HILIM
      REAL*8 INLB(NFG), INRB(NFG), ITBL, IERED(NCL), IERR
      REAL*8 INTB(NANG,NFG,NCL + 1), INT(NANG,NFG,NCL), IZIN(NFG,NCL)
      REAL*8 ITRB, ITER(NFG,NCL)
      REAL*8 L, LFL, LOWLIM
      REAL*8 MAXT
      REAL*8 NATE(NCL), NINT(NANG,NFG,NCL)
      REAL*8 NPFT(NANG,NFG,NCL), NDIN(NFG,NCL + 1), NZIN(NFG,NCL)
      REAL*8 PMA(NCL), PINT(NANG,NFG,NCL), PRTIME
      REAL*8 PGRN(NCL + 1), PFG(NCL + 1), PLANK(NFG,NCL)
      REAL*8 Q(NANG,NFG,NCL)
      REAL*8 SPH, SIG, SPR
      REAL*8 SIGM(NFG,NCL), GRS(NCL + 1)
      REAL*8 SOLU(NCL + 1), SPRB
      REAL*8 S(NFG,NCL), SUM1, SUM2, GRFQ(NCL), GRZQ(NCL)
      REAL*8 TTIME, TOU, TERR, TELB
      REAL*8 TRNFVR(NCL), TEMP(NCL)
      REAL*8 UFL
      REAL*8 WF(NANG)
      REAL*8 ZLP(NANG), ZINT(NFG,NCL), ZQ(NFG,NCL), DIER
```

```
      COMMON /R01/ ALFA, AC, ATMASS, DAF, ATEM
      COMMON /R02/ ABC, AB, AO
      COMMON /R03/ BETA, BO
      COMMON /R04/ CV, CW, CHI
      COMMON /R05/ DL, DINT, PRNTM
      COMMON /R06/ DIST, DTIME, DISPR
      COMMON /R07/ ETA
      COMMON /R08/ FR, FQ
      COMMON /R09/ HILIM
      COMMON /R10/ INLB, INRB, ITSL, IERED, IERR
      COMMON /R11/ INTB, IINT, IZIN
      COMMON /R12/ ITRB, ITER
      COMMON /R13/ L, LFL, LOWLIM
      COMMON /R14/ MAXT
      COMMON /R15/ NATE, NINT
      COMMON /R16/ NFFT, NDIN, NZIN
      COMMON /R17/ PMAC, PINT, PRTIME
      COMMON /R18/ PQIN, PFQI, PLANK
      COMMON /R19/ Q
      COMMON /R20/ SPH, SIRC, SPR
      COMMON /R21/ SIGM, GRSI
      COMMON /R22/ SOLU, SPRB
      COMMON /R23/ S, SUM1, SUM2, GRFQ, GRZQ
      COMMON /R24/ TTIME, TOU, TERR, TELB
      COMMON /R25/ TRNFVR, TEMP
      COMMON /R26/ UFL
      COMMON /R27/ WF
      COMMON /R28/ ZLP, ZINT, ZQ, DIER

      REAL*8 SPLNK(NCL), ABB(NCL), DIFRD(NCL)
      REAL*8 SUMCH(NCL), CHB(NCL), RESSIG, RESPLN
      REAL*8 PLNINT(NFQ,NCL), SIGINT(NFQ,NCL), SGPLN(NFQ,NCL)
      EXTERNAL FPLNK, F2, F3, FSIG
      INTRINSIC ALOG10, EXP
C
CL      C2.8 NON-LTE DATA FOR AVRG-Z,RADIATIVE COOLING ETC...
C   VERSION JUNE 1986 Y.T. LEE
      COMMON /LEEDRY/ HNUEDG(64), DTEMP(19), DDENS(22), ENION(19,22),
     1     TBLZ(19,22), TBLZSQ(19,22), POWER(19,22,64),
     2     SIGMA(19,22,64), HNUMIN, HNUMAX, ZATOM, NT, NR, NGHIGH,
     3     NGLOW, NORMAX, NTMAX
C
      IF (TOIT .EQ. 0) THEN
C***** define the frequency groups and the cell width ,initial temp-
C***** erature, specific heat for the model problem - only once
        DIS = 0.0
        IF (UBC .EQ. 0) THEN
C***** take uniformly spaced spatial cells
          CW = L / NC
          DIST(1) = CW / 2
          DO 10 K = 2, NC
            DIST(K) = DIST(K - 1) + CW
   10     CONTINUE
          DO 20 K = 1, NC
            DL(K) = CW
   20     CONTINUE
        END IF
C***** frequency spectrum is logarithmically grouped
        LLFL = LOG(LFL)
        LUFL = LOG(UFL)
        LFIN = (LUFL - LLFL) / NG
        LFR(1) = LLFL
        DO 30 J = 2, NG + 1
          LFR(J) = LFR(J - 1) + LFIN
   30   CONTINUE
        DO 40 J = 1, NG + 1
          FR(J) = EXP(LFR(J))
   40   CONTINUE
        DO 50 K = 1, NC
C***** specific heat is taken to be uniform in the model
          CV(K) = SPH
   50   CONTINUE
C***** define initial temperature distribution
        IF (TEMEXP .EQ. 0) THEN
C***** let initial temperature to be exponential from left to right from
C***** 1 Kev to 1 ev
          LITLB = LOG(TELB)
          DO 60 K = 1, NC
            TEMP(K) = TELB * EXP((-LITLB*(DIST(K) - DIST(K)/2))/L - (
     1      DIST(K)/2)))
   60     CONTINUE
        ELSE
C***** take initial temperature to be uniform
          DO 70 K = 1, NC
            TEMP(K) = ITSL
   70     CONTINUE
        END IF
        END IF
        IF (CONT .EQ. 0) THEN
        IF ( .NOT. SIMRUN) THEN
          TTIME = TTIME + DTIME
          IF (TTIME .GT. MAXT .AND. TOIT .NE. 0) THEN
            WRITE (*,*)'time sensitive', TTIME - DTIME, SIMRUN
            WRITE (6,*)'program terminated, must reached'
            STOP
          END IF
        END IF
        TOU = 1 / (SP*DTIME)
        IF (NFFC .EQ. 0) THEN
C***** take intensity at cell boundary to be zero when it is negative
C     TRNFVR determines the type of modification to be used for
C***** the negative flux fix up
          DO 80 K = 1, NC
            TRNFVR(K) = 0.5
   80     CONTINUE
          TRNFV = (SP*DTIME) / DL(1)
```

```
        ELSE IF (NFFC .EQ. 1) THEN
C***** take intensity at cell boundary to be cell average intensity
C***** when it is negative
          DO 90 K = 1, NC
            TRNFVR(K) = 2.0
   90     CONTINUE
          TRNFV = (SP*DTIME) / DL(1)
        ELSE IF (NFFC .EQ. 2) THEN
C***** implement negative flux fixup as shown in the thesis
          DO 100 K = 1, NC
            TRNFVR(K) = (SP*DTIME) / DL(K)
  100     CONTINUE
        END IF
        END IF
          IF (CONT .EQ. 0) THEN
        IF (TIT .GE. 1) THEN
          DO 110 K = 1, NC
            TEMP(K) = NATE(K)
  110     CONTINUE
        END IF
        DO 130 K = 1, NC
          DO 120 J = 1, NG + 1
            FF(J,K) = FR(J) / TEMP(K)
  120     CONTINUE
  130   CONTINUE
        IF (TRIN .EQ. 0 .OR. TOIT .EQ. 0) THEN
          IF (WFN .EQ. 0) THEN
C***** calculate initial intensity assuming planckian distribution
            DO 160 K = 1, NC
              DO 150 J = 1, NG
                D = FF(J,K)
                E = FF(J + 1,K)
                IF (D .GT. LOWLIM) THEN
                  D = LOWLIM
                END IF
                IF (E .GT. HILIM) THEN
                  E = HILIM
                END IF
                CALL ROMB(FPLNK, D, E, RESPLN)
C*****            WRITE (6,*)'res1 ', RESPLN
                PLANK(J,K) = (2/(SP**2)) * (TEMP(K)**4) * (BK*TCF) *
     1            RESPLN / (A0**3)
                DO 140 I = 1, NA
                  IINT(I,J,K) = (2/(SP**2)) * (TEMP(K)**4) * (BK*TCF) *
     1              RESPLN / (A0**3)
                  PINT(I,J,K) = IINT(I,J,K)
  140           CONTINUE
  150         CONTINUE
  160       CONTINUE
          ELSE
C***** calculate initial intensity assuming Rosseland distribution
            DO 190 K = 1, NC
              DO 180 J = 1, NG
                D = FF(J,K)
                E = FF(J + 1,K)
                IF (D .GT. LOWLIM) THEN
                  D = LOWLIM
                END IF
                IF (E .GT. HILIM) THEN
                  E = HILIM
                END IF
C>>>            CALL ROMB(F2, D, E, RES2)
                CALL ROMB(F3, D, E, RES3)
C*****          CALL ROMB(FPLNK, D, E, RESPLN)
                PLANK(J,K) = 1.606528E-20 * AC * RES3 * (TEMP(K)**6)
C*****          WRITE (6,*)'res2 and res3 ', RES2, RES3 , PLANK(J,K)
                DO 170 I = 1, NA
                  IINT(I,J,K) = PLANK(J,K)
                  PINT(I,J,K) = IINT(I,J,K)
  170           CONTINUE
  180         CONTINUE
  190       CONTINUE
          END IF
        ELSE
C***** take initial intensity to be the intensity from transfer equation
          DO 220 K = 1, NC
            DO 210 J = 1, NG
              DO 200 I = 1, NA
                IINT(I,J,K) = NINT(I,J,K)
                PINT(I,J,K) = IINT(I,J,K)
  200         CONTINUE
  210       CONTINUE
  220     CONTINUE
        END IF
        DO 230 J = 1, NG
          DO 240 K = 1, NC
            ZINT(J,K) = 0.0
            DO 230 I = 1, NA
              ZINT(J,K) = ZINT(J,K) + IINT(I,J,K) * WF(I)
  230       CONTINUE
            IZIN(J,K) = ZINT(J,K)
  240     CONTINUE
  250   CONTINUE
        DO 270 K = 1, NC
          SPLNK(K) = 0.0
          DO 260 J = 1, NG
            D = FF(J,K)
            E = FF(J + 1,K)
            IF (D .GT. LOWLIM) THEN
              D = LOWLIM
            END IF
            IF (E .GT. HILIM) THEN
              E = HILIM
            END IF
            CALL ROMB(FPLNK, D, E, RESPLN)
            SPLNK(K) = SPLNK(K) + RESPLN
```

```
      260   CONTINUE
      270  CONTINUE
           DO 280 K = 1, NC
            IERED(K) = 4 * PI * 5.03343E+07 * SPLNK(K) / SP
      280  CONTINUE
           IF (PRES .GE. 5 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
          1   THEN
            WRITE (8,290) (K,DL(K),CV(K),TEMP(K)/11604,IERED(K),K=1,NC)
      290   FORMAT (2(/I',I2,1X,'dl=',1PE10.3,1X,'cv=',1PE10.3,1X,'temp=',
          1    1PE10.3,1X,'ie=',1PE10.3,1X))
            WRITE (8,*)'freq group limits model'
            WRITE (8,300) (J,FR(J),J=1,NG + 1)
      300   FORMAT (/8('g',I2,1X,F11.4,1X))
            WRITE (8,*)' k ext m model'
            WRITE (8,310) (((J,K,IENT(J,JK),K=1,NC),J=1,NG),J=1,NA)
      310   FORMAT (/6('/',I2,1X,'j',I2,1X,'k',I2,1X,1PE10.3,1X))
            WRITE (8,*)' k zint model'
            WRITE (8,320) ((J,K,ZINT(J,K),K=1,NC),J=1,NG)
      320   FORMAT (/8(I2,1X,I2,1X,1PE10.3,1X))
            WRITE (8,*)' k integration limits model'
            WRITE (8,330) ((J,K,FF(J,K),K=1,NC),J=1,NG + 1)
      330   FORMAT (/8(I2,1X,I2,1X,1PE10.3))
           END IF
          END IF
          IF (CONT .EQ. 1) THEN
C**** solve opacity at new temp.
           GO TO 400
          END IF
          IF (TTIME .GE. 1.0005E-10 .AND. TOIT .NE. 0) THEN
C**** no need to calculate intensity at the boundary, save temperature
C**** rewrite constant after 0.1 ns for time dependent case.
           GO TO 400
          END IF
          IF (TEMPTD .EQ. 0) THEN
C**** express temperature on left and as linear function of time
C**** until it reaches its maximum value (1000 ev)
           IF (TTIME .LT. 1.00005E-10) THEN
            ITLB = ((TELB - 1)*TTIME/1.0E-10 + 1)
           ELSE
            ITLB = TELB
           END IF
          ELSE
           ITLB = TELB
          END IF
          WRITE (6,*)'itlb itrb', ITLB, ITRB
          DO 340 J = 1, NG
           D = FR(J) / ITLB
           E = FR(J + 1) / ITLB
           IF (D .GT. LOWLIM) THEN
            D = LOWLIM
           END IF
           IF (E .GT. HILIM) THEN
            E = HILIM
           END IF
           CALL ROMB(FPLNK, D, E, RESPLN)
C          WRITE (6,280) J, RESPLN
C 280   FORMAT (1X, 'J = ', I2, 2X, 'INTEGRAL INLB = ', 1PE10.3)
           INLB(J) = (2/(SP**2)) * (ITLB**4) * (BK*TCF) * RESPLN / (A0**3)
      340 CONTINUE
          DO 350 J = 1, NG
           D = FR(J) / ITRB
           E = FR(J + 1) / ITRB
           IF (D .GT. LOWLIM) THEN
            D = LOWLIM
           END IF
           IF (E .GT. HILIM) THEN
            E = HILIM
           END IF
           CALL ROMB(FPLNK, D, E, RESPLN)
C          WRITE (6,300) J, RESPLN
C 300   FORMAT (1X, 'J = ', I2, 2X, 'INTEGRAL INRB = ', 1PE10.3)
           INRB(J) = (2/(SP**2)) * (ITRB**4) * (BK*TCF) * RESPLN / (A0**3)
      350 CONTINUE
          IF (RETSOU .EQ. 0) THEN
C****  no source on the right boundary
           DO 360 J = 1, NG
            INRB(J) = 0.0
      360   CONTINUE
          ELSE IF (RETSOU .EQ. 1) THEN
C****  no source on the left or right boundary
           DO 370 J = 1, NG
            INLB(J) = 0.0
            INRB(J) = 0.0
      370   CONTINUE
          END IF
          IF (PRES .GE. 1.0 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
          1   THEN
           WRITE (8,380) ITLB, ITRB
      380   FORMAT (1X, 'ITLB = ', 1PE10.3, 1X, 'ITRB = ', 1PE10.3)
           WRITE (8,390) (J,INLB(J),INRB(J),J=1,NG)
      390   FORMAT (4(/',I2,1X,2(1PE10.3,1X)))
          END IF
      400 IF (TIT .LT. 1) THEN
           DO 410 K = 1, NC
            ATEM(K) = TEMP(K)
      410   CONTINUE
          END IF
          DO 430 K = 1, NC
           DO 420 J = 1, NG + 1
            FF(J,K) = FR(J) / ATEM(K)
      420   CONTINUE
      430 CONTINUE
          IF (WFN .EQ. 0) THEN
           DO 450 K = 1, NC
            SPLNK(K) = 0.0
            ABB(K) = 0.0
```

127

```
           DO 440 J = 1, NG
            D = FF(J,K)
            E = FF(J + 1,K)
            IF (D .GT. LOWLIM) THEN
             D = LOWLIM
            END IF
            IF (E .GT. HILIM) THEN
             E = HILIM
            END IF
            CALL ROMB(FPLNK, D, E, RESPLN)
            CALL ROMB(FSIG, D, E, RESSIG)
            PLNINT(J,K) = RESPLN
            SIGINT(J,K) = RESSIG
            SPLNK(K) = SPLNK(K) + PLNINT(J,K)
            ABB(K) = ABB(K) + PLNINT(J,K) * SIGINT(J,K)
            SOPLN(J,K) = (EXP(-D) - EXP(-E))
      440   CONTINUE
      450  CONTINUE
           DO 470 K = 1, NC
            DO 460 J = 1, NG
             CH(J,K) = SIGINT(J,K) * PLNINT(J,K) / ABB(K)
             ABC(J,K) = 27.0 * AC * SOPLN(J,K) / ((ATEM(K)**3)*PLNINT(J,
          1   K))
      460   CONTINUE
      470  CONTINUE
           ELSE
            DO 490 K = 1, NC
             SPLNK(K) = 0.0
             ABB(K) = 0.0
             DO 480 J = 1, NG
              D = FF(J,K)
              E = FF(J + 1,K)
              IF (D .GT. LOWLIM) THEN
               D = LOWLIM
              END IF
              IF (E .GT. HILIM) THEN
               E = HILIM
              END IF
              CH(J,K) = (EXP(-D) - EXP(-E))
              CALL ROMB(F2, D, E, RES2)
              CALL ROMB(F3, D, E, RES3)
              CALL ROMB(FPLNK, D, E, RESPLN)
              CALL ROMB(FSIG, D, E, RESSIG)
              PLNINT(J,K) = RESPLN
              SIGINT(J,K) = RESSIG
              SPLNK(K) = SPLNK(K) + PLNINT(J,K)
              ABB(K) = ABB(K) + PLNINT(J,K) * SIGINT(J,K)
              SOPLN(J,K) = (EXP(-D) - EXP(-E))
C             WRITE (6,*)'res2 and res3 ', RES2, RES3
      480    CONTINUE
      490   CONTINUE
            DO 510 K = 1, NC
             DO 500 J = 1, NG
              CH(J,K) = SIGINT(J,K) * PLNINT(J,K) / ABB(K)
              ABC(J,K) = 27.0 * (AC) * RES2 / ((ATEM(K)**3)*RES3)
      500    CONTINUE
      510   CONTINUE
            END IF
            DO 520 K = 1, NC
             PMAC(K) = 27.0 * AC * ABB(K) / ((ATEM(K)**3)*SPLNK(K))
             BETA(K) = 4 * BK * ((ATEM(K)*TCF)**3) / CV(K)
             ALFA(K) = 1 / (PMAC(K)*BETA(K))
      520 CONTINUE
            DO 530 K = 1, NC
             ETA(K) = 1 / (1 + ALFA(K)*TOU)
             DIFFRD(K) = SPLNK(K) * 4 * PI / SP
      530 CONTINUE
            SRC = 0.0
            DO 540 K = 1, NC
             SRC = SRC + ETA(K)
      540 CONTINUE
            SRC = SRC / NC
            IF (PRES .GE. 2 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
          1   THEN
             WRITE (8,*)'beta pmac alfa in model'
             WRITE (8,550) (K,BETA(K),PMAC(K),ALFA(K),K=1,NC)
      550   FORMAT (3(I2,1X,3(1PE10.3,1X)))
            END IF
            DO 580 J = 1, NG
             DO 570 K = 1, NC
              PQ(J,K) = 0.0
              DO 560 I = 1, NA
               Q(J,K) = CH(J,K) * IERED(K) * ETA(K) / (2*DTIME*BETA(K))
          1    + TOU * ENT(J,K)
               PQ(J,K) = PQ(J,K) + ENT(J,K) * WF(I) * ZLP(I)
      560    CONTINUE
             SIGMA(J,K) = (ABC(J,K) + TOU) * DL(K)
             ZQ(J,K) = CH(J,K) * IERED(K) * ETA(K) / (DTIME*BETA(K)) +
          1   TOU * ZINT(J,K)
      570   CONTINUE
      580 CONTINUE
            DO 600 K = 1, NC
             GRZQ(K) = 0.0
             GRPQ(K) = 0.0
             SUMCH(K) = 0.0
             DO 590 J = 1, NG
              GRZQ(K) = GRZQ(K) + ZQ(J,K)
              GRPQ(K) = GRPQ(K) + PQ(J,K) / SIGMA(J,K)
              SUMCH(K) = SUMCH(K) + CH(J,K)
      590    CONTINUE
      600 CONTINUE
            IF (PRES .GE. 2 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
          1   THEN
             WRITE (8,*)'sum of chis and sbbchi model'
             WRITE (8,610) (K,SUMCH(K),ABB(K),K=1,NC)
      610   FORMAT (3(I2,1X,2(1PE11.4,1X)))
```

```
      WRITE (8,*)'j k chi sbc plank to model'
      WRITE (8,620) ((J,K,CHI(J,K),ABC(J,K),PLANK(J,K),J=1,NG),K=1,NC)
  620 FORMAT (3(I2,1X,I2,1X,3(1PE10.3,1X)))
      WRITE (8,*)' i j k q model'
      WRITE (8,630) (((J,K,Q(J,J,K),K=1,NC),J=1,NG),J=1,NA)
  630 FORMAT (6(I2,1X,I2,1X,I2,1X,1PE10.3,1X))
      PAUSE
      END IF
      IF (TIT .GE. 1) THEN
       DO 660 J = 1, NG
        DO 650 K = 1, NC
         ZINT(J,K) = 0.0
         DO 640 I = 1, NA
          ZINT(J,K) = ZINT(J,K) + NINT(I,J,K) * WF(I)
  640    CONTINUE
  650   CONTINUE
  660  CONTINUE
       END IF
       DO 680 K = 1, NC
        AB(K) = 0.0
        DO 670 J = 1, NG
         AB(K) = AB(K) + ABC(J,K) * ZINT(J,K)
  670  CONTINUE
  680 CONTINUE
      IF (PRES .GE. 2 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1   THEN
       WRITE (8,*)'j k zint zq model'
       WRITE (8,690) ((J,K,ZINT(J,K),ZQ(J,K),J=1,NG),K=1,NC)
  690  FORMAT (5(I2,1X,I2,1X,1PE10.3,1X,1PE10.3))
      END IF
      RETURN
      END
C
C  ***************************************************************************
C  *  this subroutine solves the RTE equation and evaluates the  *
C  * the variable needed for solving the diffusion equation      *
C  ***************************************************************************
C
      SUBROUTINE TRNFRT

      PARAMETER (NANG=24,NFG=64,NCL=151)
      PARAMETER (SP=3.0E08)

      INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      INTEGER DRT, DIFBC, DIFACC, IIT, TITA
      INTEGER INSB, IRUN, LIN, MEDUSA
      INTEGER NA, NG, NC, NF, NDIT, NFFC, NDICNT, NFMUST
      INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      INTEGER USC, WFN, CONV, DBXL, DBXU, NUM
      INTEGER NCP1, NCM1, NAD2

      COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      COMMON /I2/ DRT, DIFBC, DIFACC, IIT, TITA
      COMMON /I3/ INSB, IRUN, LIN, MEDUSA
      COMMON /I4/ NA, NG, NC, NF, NDIT, NFFC, NDICNT, NFMUST
      COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      COMMON /I7/ USC, WFN, CONV, DBXL, DBXU, NUM
      COMMON /I8/ NCP1, NCM1, NAD2

      REAL*8 ALFA(NCL), AC, ATMASS, DAF(NFG,NCL), ATEM(NCL)
      REAL*8 ABC(NFG,NCL), AB(NCL), AO(NFG,NCL)
      REAL*8 BETA(NCL), BO(NFG,NCL)
      REAL*8 CV(NCL), CW, CH(NFG,NCL)
      REAL*8 DL(NCL), DINT(NFG,NCL + 1), PRNTM
      REAL*8 DIST(NCL), DTIME, DEPR
      REAL*8 ETA(NCL)
      REAL*8 FINT(NFG,NCL + 1), FINL(NFG), FINR(NFG)
      REAL*8 FR(NFG + 1), FQ(NFG,NCL)
      REAL*8 INLB(NFG), INRB(NFG), ITSL, SERED(NCL), ZERR
      REAL*8 INTB(NANG,NFG,NCL + 1), INT(NANG,NFG,NCL), IZIN(NFG,NCL)
      REAL*8 ITRB, ITER(NFG,NCL)
      REAL*8 NATE(NCL), NINT(NANG,NFG,NCL)
      REAL*8 NFFT(NANG,NFG,NCL), NDIN(NFG,NCL + 1), NZIN(NFG,NCL)
      REAL*8 PMAC(NCL), PINT(NANG,NFG,NCL), PRTIME
      REAL*8 PQIN(NCL + 1), PFQI(NCL + 1), PLANK(NFG,NCL)
      REAL*8 PDIN(NFG,NCL + 1), PITE(NFG,NCL), PZIN(NFG,NCL)
      REAL*8 PABO(NCL)
      REAL*8 QQ(NANG,NFG,NCL)
      REAL*8 SIGM(NFG,NCL), GRSI(NCL + 1)
      REAL*8 SQ(NFG,NCL), SUM1, SUM2, ORFQ(NCL), GRZQ(NCL)
      REAL*8 SINT(NFG,NCL + 1)
      REAL*8 TTIME, TOU, TERR, TELB
      REAL*8 TRNFVR(NCL), TEMP(NCL)
      REAL*8 WF(NANG)
      REAL*8 ZLP(NANG), ZINT(NFG,NCL), ZQ(NFG,NCL), DIER

      COMMON /R01/ ALFA, AC, ATMASS, DAF, ATEM
      COMMON /R02/ ABC, AB, AO
      COMMON /R03/ BETA, BO
      COMMON /R04/ CV, CW, CH
      COMMON /R05/ DL, DINT, PRNTM
      COMMON /R06/ DIST, DTIME, DEPR
      COMMON /R07/ ETA
      COMMON /R071/ FINT, FINL, FINR
      COMMON /R08/ FR, FQ
      COMMON /R10/ INLB, INRB, ITSL, SERED, ZERR
      COMMON /R11/ INTB, INT, IZIN
      COMMON /R12/ ITRB, ITER
      COMMON /R15/ NATE, NINT
      COMMON /R16/ NFFT, NDIN, NZIN
      COMMON /R17/ PMAC, PINT, PRTIME
      COMMON /R18/ PQIN, PFQI, PLANK
      COMMON /R181/ PDIN, PITE, PZIN
      COMMON /R182/ PAB

      COMMON /R19/ Q
      COMMON /R21/ SIGM, GRSI
      COMMON /R23/ S, SUM1, SUM2, ORFQ, GRZQ
      COMMON /R231/ SINT
      COMMON /R24/ TTIME, TOU, TERR, TELB
      COMMON /R25/ TRNFVR, TEMP
      COMMON /R27/ WF
      COMMON /R28/ ZLP, ZINT, ZQ, DIER

      COMMON /IMT/ I, N

      DO 60 I = 1, NAD2
       DO 50 J = 1, NG
        DO 40 K = 1, NC
         NFFT(I,J,K) = 0.0
         INTB(I,J,1) = INLB(J)
         NINT(I,J,K) = (((CHI(J,K)*ETA(K)*AB(K))/2 + Q(I,J,K))*DL(K) +
     1   2*ZLP(I)*INTB(I,J,K)) / (SIGM(J,K) + 2*ZLP(I))
         INTB(I,J,K + 1) = 2 * NINT(I,J,K) - INTB(I,J,K)
         IF (PRES .GE. 15 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1      THEN
          WRITE (8,10) I, J, K, PINT(I,J,K), NINT(I,J,K),
     1    NINT(I,J,K) / PINT(I,J,K), INTB(I,J,K + 1)
     10   FORMAT (1X, 'I J K PI NI NI/P INTB=', 3(I2,1X),
     1       4(1PE10.3,1X))
         END IF
C**** negative flux fix up criterion is selected (63), according
C**** to TRNFVR value
         IF (NF .EQ. 0) THEN
          IF (INTB(I,J,K + 1) .LT. 0) THEN
           NFFT(I,J,K) = 1.0
           COUNT = COUNT + 1
           IF (TRNFVR(K) .LT. 1) THEN
            NINT(I,J,K) = (((CHI(J,K)*ETA(K)*AB(K))/2 + Q(I,J,K))*
     1      DL(K) + ZLP(I)*INTB(I,J,K)) / SIGM(J,K)
            INTB(I,J,K + 1) = 0.0
            IF (PRES .GE. 15 .AND. TOIT .GE. DBXL .AND. TOIT .LE.
     1         DBXU) THEN
             WRITE (8,20) I, J, K, PINT(I,J,K), NINT(I,J,K),
     1       NINT(I,J,K) / PINT(I,J,K), INTB(I,J,K + 1)
     20      FORMAT (1X, 'I J K PI NI NI/P INTB=', 3(I2,1X),
     1          4(1PE10.3,1X))
            END IF
           ELSE
            NINT(I,J,K) = (((CHI(J,K)*ETA(K)*AB(K))/2 + Q(I,J,K))*
     1      DL(K) + ZLP(I)*INTB(I,J,K)) / (SIGM(J,K) + ZLP(I))
            INTB(I,J,K + 1) = NINT(I,J,K)
            IF (PRES .GE. 15 .AND. TOIT .GE. DBXL .AND. TOIT .LE.
     1         DBXU) THEN
             WRITE (8,30) I, J, K, PINT(I,J,K), NINT(I,J,K),
     1       NINT(I,J,K) / PINT(I,J,K), INTB(I,J,K + 1)
     30      FORMAT (1X, 'I J K PI NI NI/P INTB=', 3(I2,1X),
     1          4(1PE10.3,1X))
            END IF
           END IF
          END IF
  40    CONTINUE
  50   CONTINUE
  60  CONTINUE
       DO 120 I = NAD2 + 1, NA
        DO 110 J = 1, NG
         DO 100 K = NC, 1, -1
          INTB(I,J,NCP1) = INRB(J)
          NFFT(I,J,K) = 0.0
          NINT(I,J,K) = (((CHI(J,K)*ETA(K)*AB(K))/2 + Q(I,J,K))*DL(K) -
     1    2*ZLP(I)*INTB(I,J,K + 1)) / (SIGM(J,K) - 2*ZLP(I))
          INTB(I,J,K) = 2 * NINT(I,J,K) - INTB(I,J,K + 1)
          IF (PRES .GE. 15 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1       THEN
           WRITE (8,70) I, J, K, PINT(I,J,K), NINT(I,J,K),
     1     NINT(I,J,K) / PINT(I,J,K), INTB(I,J,K)
     70    FORMAT (1X, 'I J K PI NI NI/P INTB=', 3(I2,1X),
     1        4(1PE10.3,1X))
          END IF
C**** negative flux fix up criterion is selected, according to
C**** TRNFVR value.
          IF (NF .EQ. 0) THEN
           IF (INTB(I,J,K) .LT. 0) THEN
            NFFT(I,J,K) = 1.0
            COUNT = COUNT + 1
            IF (TRNFVR(K) .LT. 1) THEN
             NINT(I,J,K) = (((CHI(J,K)*ETA(K)*AB(K))/2 + Q(I,J,K))*
     1       DL(K) - ZLP(I)*INTB(I,J,K + 1)) / SIGM(J,K)
             INTB(I,J,K) = 0.0
             IF (PRES .GE. 15 .AND. TOIT .GE. DBXL .AND. TOIT .LE.
     1          DBXU) THEN
              WRITE (8,80) I, J, K, PINT(I,J,K), NINT(I,J,K),
     1        NINT(I,J,K) / PINT(I,J,K), INTB(I,J,K)
     80       FORMAT (1X, 'I J K PI NI NI/P INTB=', 3(I2,1X),
     1           4(1PE10.3,1X))
             END IF
            ELSE
             NINT(I,J,K) = (((CHI(J,K)*ETA(K)*AB(K))/2 + Q(I,J,K))*
     1       DL(K) - ZLP(I)*INTB(I,J,K + 1)) / (SIGM(J,K) - ZLP(I))
             INTB(I,J,K) = NINT(I,J,K)
             IF (PRES .GE. 15 .AND. TOIT .GE. DBXL .AND. TOIT .LE.
     1          DBXU) THEN
              WRITE (8,90) I, J, K, PINT(I,J,K), NINT(I,J,K),
     1        NINT(I,J,K) / PINT(I,J,K), INTB(I,J,K)
     90       FORMAT (1X, 'I J K PI NI NI/P INTB=', 3(I2,1X),
     1           4(1PE10.3,1X))
             END IF
            END IF
           END IF
```

```
      100   CONTINUE
      110   CONTINUE
      120 CONTINUE
          DO 150 J = 1, NG
          DO 140 K = 1, NCP1
            DINT(J,K) = 0.0
            DO 130 I = 1, NA
              DINT(J,K) = DINT(J,K) + INTB(J,K) * WF(I)
      130   CONTINUE
      140   CONTINUE
      150 CONTINUE
          IF (PRES .GE. 2) THEN
            WRITE (8,160) (((J,K,PINT(J,K),NINT(J,K),J=1,NA),J=1,NG),
     1    K=1,NC)
      160   FORMAT (3(3(I2,1X),2(1PE10.3,1X)))
          END IF
          IF (TRNACC .EQ. 1) THEN
            DO 190 J = 1, NG
              DO 180 K = 1, NCP1
                DINT(J,K) = 0.0
                PINT(J,K) = 0.0
                SINT(J,K) = 0.0
                DO 170 I = 1, NA
                  DINT(J,K) = DINT(J,K) + INTB(J,K) * WF(I)
                  PINT(J,K) = PINT(J,K) + INTB(J,K) * ZLP(I) * WF(I)
                  SINT(J,K) = SINT(J,K) + INTB(J,K) * WF(I) * (3 *ZLP(I)**
     1            2 - 1) / 2
      170         CONTINUE
                PDIN(J,K) = DINT(J,K)
      180       CONTINUE
      190     CONTINUE
            DO 220 K = 1, NC
              DO 210 J = 1, NG
                ZINT(J,K) = 0.0
                PZIN(J,K) = 0.0
                DO 200 I = 1, NA
                  ZINT(J,K) = ZINT(J,K) + NINT(J,K) * WF(I)
                  PZIN(J,K) = PZIN(J,K) + PINT(J,K) * WF(I)
      200       CONTINUE
      210     CONTINUE
      220   CONTINUE
            DO 240 K = 1, NC
              PAB(K) = 0.0
              DO 230 J = 1, NG
                PAB(K) = PAB(K) + ABC(J,K) * PZIN(J,K)
      230     CONTINUE
      240   CONTINUE
            DO 260 K = 1, NCP1
              PFO(K) = 0.0
              PGIN(K) = 0.0
              DO 250 J = 1, NG
                PFO(K) = PFO(K) + PINT(J,K)
                PGIN(K) = PGIN(K) + DINT(J,K)
      250     CONTINUE
      260   CONTINUE
            DO 280 K = 1, NC
              GRS(K) = 0.0
              DO 270 J = 1, NG
                GRS(K) = GRS(K) + (SINT(J,K + 1) - SINT(J,K)) / SIGM(J,K)
      270     CONTINUE
      280   CONTINUE
            IF (PRES .GE. 5 .AND. TOIT .GT. DBXL .AND. TOIT .LE. DBXU)
     1        THEN
              WRITE (8,*)'k pfgi pgin'
              WRITE (8,290) (K,PFO(K),PGIN(K),K=1,NCP1)
      290     FORMAT (1X, 5(I4',2,1X,2(1PE10.3),1X))
              WRITE (8,*)'k nurm'
              WRITE (8,300) (K,GRS(K),K=1,NC)
      300     FORMAT (1X, 5(I4',2,1X,1PE10.3,1X))
            END IF
c**** negative flux fix up criterion is selected
            IF (NF .EQ. 0) THEN
              DO 330 J = 1, NG
                DO 320 K = 1, NC
                  DO 310 I = 1, NA
                    IF (NFPT(J,K) .GT. 0.5) THEN
                      IF (DINT(J,K + 1) .EQ. 0.0) THEN
                        AO(J,K) = 1.0
                      ELSE
                        AO(J,K) = ZINT(J,K) / DINT(J,K + 1)
                      END IF
                      IF (DINT(J,K) .EQ. 0.0) THEN
                        BO(J,K) = 1.0
                      ELSE
                        BO(J,K) = ZINT(J,K) / DINT(J,K)
                      END IF
                      GO TO 320
                    ELSE
                      AO(J,K) = 1.0
                      BO(J,K) = 1.0
                    END IF
      310           CONTINUE
      320         CONTINUE
      330       CONTINUE
              END IF
              DO 350 K = 1, NC
                AB(K) = 0.0
                DO 340 J = 1, NG
                  AB(K) = AB(K) + ABC(J,K) * (AO(J,K)*DINT(J,K + 1) + BO(J,K)*
     1            DINT(J,K))
      340         CONTINUE
                PAB(K) = 2 * PAB(K)
      350       CONTINUE
              IF (PRES .GE. 5 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1          THEN
                WRITE (8,*)'k ab for diff'
```

```
            WRITE (8,360) (K,AB(K),K=1,NC)
      360     FORMAT (4(1X,'k',I2,1X,1PE10.3))
            END IF
            DO 380 J = 1, NG
              DO 370 K = 1, NCM1
                S(J,K) = (DL(K)*ZQ(J,K) + DL(K + 1)*ZQ(J,K + 1)) / 2 - (
     1          PINT(J,K + 2) - PINT(J,K)) / 2 - (DINT(J,K + 2) - DINT(J,K +
     2          1)) / (3 *SIGM(J,K + 1)) + (DINT(J,K + 1) - DINT(J,K)) / (3*
     3          SIGM(J,K))
      370       CONTINUE
      380     CONTINUE
            DO 400 K = 1, NC
              DO 390 J = 1, NG
                ITER(J,K) = DL(K) * CHI(J,K) * ETA(K) * AB(K) / 4
                PITE(J,K) = DL(K) * CHI(J,K) * ETA(K) * PAB(K) / 4
      390       CONTINUE
      400     CONTINUE
            IF (PRES .GE. 7 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1        THEN
              WRITE (8,*)'toit dbxt', TOIT
              WRITE (8,*)'j k ao bo fs'
              WRITE (8,410) ((J,K,AO(J,K),BO(J,K),FQ(J,K),K=1,NC),J=1,NG)
      410     FORMAT (1X, 2(I2,1X,I2,1X,3(1PE10.3,1X)))
              WRITE (8,*)'j k s(j,k)'
              WRITE (8,420) ((J,K,S(J,K),K=1,NCM1),J=1,NG)
      420     FORMAT (1X, 4(I2,1X,I2,1X,1PE10.3,1X))
              WRITE (8,*)'k j zq sigm'
              WRITE (8,430) ((J,K,ZQ(J,K),SIGM(J,K),K=1,NC),J=1,NG)
      430     FORMAT (2(I2,1X,I2,2(1PE10.3,1X)))
              WRITE (8,*)'k j first pdin sint'
              WRITE (8,440) (J,K,PINT(J,K),PDIN(J,K),SINT(J,K),K=1,NCP1),J=
     1    1,NG)
      440     FORMAT (1X, I2, 1X, I2, 1X, 1PE10.3, 1X, 1PE10.3, 1X, 1PE10.3)
            END IF
          END IF
          RETURN
          END
c
c  ********************************************************************
c  * this subroutine computes the spectral radius and determines if   *
c  * the intensity is converged.                                      *
c  ********************************************************************
c
          SUBROUTINE TRCONV

          PARAMETER (NANG=24,NFG=64,NCL=151)

          REAL*8 DIFFF
          REAL*8 NDIF
          REAL*8 PDIF
          REAL*8 SNIN(NCL), SPIN(NCL)
          REAL*8 TINT

          INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
          INTEGER DRT, DIFBC, DIFACC, IIT, TITA
          INTEGER INSB, IRUN, LIN, MEDUSA
          INTEGER NA, NG, NC, NF, NDIT, NFFC, NDSCNT, NFMUST
          INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
          INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
          INTEGER UBC, WFN, CONV, DBXL, DBXU, NUM
          INTEGER NCP1, NCM1, NAD2
          INTEGER SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

          LOGICAL TRN, DIFF, LOR, NLOR, SIMRUN, SMTST
          COMMON /L1/ TRN, DIFF, LOR, NLOR, SIMRUN, SMTST

          COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
          COMMON /I2/ DRT, DIFBC, DIFACC, IIT, TITA
          COMMON /I3/ INSB, IRUN, LIN, MEDUSA
          COMMON /I4/ NA, NG, NC, NF, NDIT, NFFC, NDSCNT, NFMUST
          COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
          COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
          COMMON /I7/ UBC, WFN, CONV, DBXL, DBXU, NUM
          COMMON /I8/ NCP1, NCM1, NAD2
          COMMON /SMT/ SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

          REAL*8 ABC(NFG,NCL), AB(NCL), AO(NFG,NCL)
          REAL*8 DL(NCL), DINT(NFG,NCL + 1), PRNTM
          REAL*8 DIST(NCL), DTIME, DSPR
          REAL*8 FR(NFG + 1), FQ(NFG,NCL)
          REAL*8 INLB(NFG), INRB(NFG), ITSL, ISRED(NCL), ERR
          REAL*8 HILIM
          REAL*8 NATE(NCL), NINT(NANG,NFG,NCL)
          REAL*8 PMAC(NCL), PINT(NANG,NFG,NCL), PRTIME
          REAL*8 SOLU(NCL + 1), SPRB
          REAL*8 SPH, SIRC, SPR
          REAL*8 WF(NANG)

          COMMON /R02/ ABC, AB, AO
          COMMON /R05/ DL, DINT, PRNTM
          COMMON /R06/ DIST, DTIME, DSPR
          COMMON /R08/ FR, FQ
          COMMON /R09/ HILIM
          COMMON /R10/ INLB, INRB, ITSL, ISRED, ERR
          COMMON /R15/ NATE, NINT
          COMMON /R17/ PMAC, PINT, PRTIME
          COMMON /R22/ SOLU, SPRB
          COMMON /R26/ SPH, SIRC, SPR
          COMMON /R27/ WF

          IF (RT .LT. 1) THEN
            DO 30 K = 1, NC
              SNIN(K) = 0.0
              SPIN(K) = 0.0
              DO 20 J = 1, NG
                DO 10 I = 1, NA
```

```
            SPIN(K) = SPIN(K) + (ABC(J,K)*PINT(I,J,K)*WF(I)*(FR(J + 1)
     1       -FR(J)))
            SNIN(K) = SNIN(K) + (ABC(J,K)*NINT(I,J,K)*WF(I)*(FR(J + 1)
     1       -FR(J)))
   10     CONTINUE
   20     CONTINUE
   30   CONTINUE
        DIFFF = 0.0
        DO 40 K = 1, NC
          DIFFF = DIFFF + (((SNIN(K) - SPIN(K))/2)**2) * DL(K)
   40   CONTINUE
        PDIF = SQRT(DIFFF/4)
        NDIF = PDIF
        RT = 2
        GO TO 110
       ELSE
        DO 70 K = 1, NC
         SNIN(K) = 0.0
         DO 60 J = 1, NG
          DO 50 I = 1, NA
           SNIN(K) = SNIN(K) + (ABC(J,K)*NINT(I,J,K)*WF(I)*(FR(J + 1)
     1       -FR(J)))
   50     CONTINUE
   60     CONTINUE
   70   CONTINUE
        DIFFF = 0.0
        DO 80 K = 1, NC
          DIFFF = DIFFF + (((SNIN(K) - SPIN(K))/2)**2) * DL(K)
   80   CONTINUE
        NDIF = SQRT(DIFFF/4)
       END IF
       SPR = NDIF / PDIF
       PDIF = NDIF
       IF (PRES .GE. 2) THEN
          WRITE (6,90) TOIT, TIIT, TIT
   90   FORMAT (1X, 'TOIT=', 1E, 3X, 'TIIT=', 1E, 3X, 'TIT=', 1E)
        WRITE (6,100) NDIF, SPR, SERC, DSPR
  100   FORMAT (1X, 'INTE ERR=', 1PE10.3, 3X, 'TRAN SPR=', 1PE10.5, 3X,
     1       'SERC=', 1PE10.3, 3X, 'DSPR=', 1PE10.3)
       END IF
       IF (SPR .GE. 1.00) THEN
        SMTST1 = SMTST1 + 1
        IF (SMTST1 .GE. 5) THEN
         WRITE (8,*)'transport terminated due to large spr'
         SMTST = .TRUE.
        END IF
       END IF
  110 DO 120 K = 1, NC
        SPIN(K) = SNIN(K)
  120 CONTINUE
       IF (CONVC .EQ. 0) THEN
        IF (NDIF .GE. ERR) GO TO 210
        CONV = 1
       ELSE IF (CONVC .EQ. 1) THEN
        DO 150 J = 1, NG
         DO 140 K = 1, NC
          DO 130 I = 1, NA
           IF (ABS((NINT(I,J,K) - PINT(I,J,K))/PINT(I,J,K)) .GE.
     1       ERR) GO TO 210
  130     CONTINUE
  140    CONTINUE
  150   CONTINUE
       ELSE IF (CONVC .EQ. 2) THEN
        DO 200 K = 1, NC
         TINT = 0.0
         DO 170 J = 1, NG
          DO 160 I = 1, NA
           TINT = TINT + PINT(I,J,K)
  160     CONTINUE
  170    CONTINUE
         DO 190 J = 1, NG
          DO 180 I = 1, NA
           IF (ABS((NINT(I,J,K) - PINT(I,J,K))/TINT) .GE. ERR)
     1       GO TO 210
  180     CONTINUE
  190    CONTINUE
  200   CONTINUE
       END IF
       CONV = 0
       RETURN
  210 CONV = 1
       IF (AUTACL .EQ. 1) THEN
        IF (SPR .GT. SPRB .AND. DSPR .LT. 0.80) THEN
         TRNACC = 1
         DIFACC = 2
        ELSE
         TRNACC = 0
        END IF
       END IF
       RETURN
       END
C
C  ***************************************************************
C  * following subroutine computes the iterative term used to    *
C  * solve the transfer equation using SI.                       *
C  ***************************************************************
C
      SUBROUTINE TRNSI

      PARAMETER (NANG=24,NFG=64,NCL=151)

      INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      INTEGER DRT, DIFBC, DIFACC, IIT, TITA
      INTEGER INSB, IRUN, LIN, MEDUSA
      INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      INTEGER USC, WFN, CONV, DBXL, DBXU, NUM
      INTEGER NCP1, NCM1, NAD2
      INTEGER SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

      COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      COMMON /I2/ DRT, DIFBC, DIFACC, IIT, TITA
      COMMON /I3/ INSB, IRUN, LIN, MEDUSA
      COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      COMMON /I7/ USC, WFN, CONV, DBXL, DBXU, NUM
      COMMON /I8/ NCP1, NCM1, NAD2
      COMMON /SMT/ SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

      REAL*8 ALFA(NCL), AC, ATMASS, DAF(NFG,NCL), ATEM(NCL)
      REAL*8 ABC(NFG,NCL), AB(NCL), AO(NFG,NCL)
      REAL*8 BETA(NCL), BO(NFG,NCL)
      REAL*8 CV(NCL), CW, CH(NFG,NCL)
      REAL*8 DL(NCL), DINT(NFG,NCL + 1), PRNTM
      REAL*8 DIIT(NCL), DTIME, DSPR
      REAL*8 ETA(NCL)
      REAL*8 FINT(NFG,NCL + 1), FINL(NFG), FINR(NFG)
      REAL*8 FR(NFG + 1), FQ(NFG,NCL)
      REAL*8 INTR(NANG,NFG,NCL + 1), INT(NANG,NFG,NCL), IZIN(NFG,NCL)
      REAL*8 ITRB, ITER(NFG,NCL)
      REAL*8 NATE(NCL), NINT(NANG,NFG,NCL)
      REAL*8 NPFT(NANG,NFG,NCL), NDIN(NFG,NCL + 1), NZIN(NFG,NCL)
      REAL*8 PMAC(NCL), PINT(NANG,NFG,NCL), PRTIME
      REAL*8 PQIN(NCL + 1), PFG(NCL + 1), PLANK(NFG,NCL)
      REAL*8 PZIN(NFG,NCL + 1), PITR(NFG,NCL), PZIN(NFG,NCL)
      REAL*8 SIGM(NFG,NCL), GRIZ(NCL + 1)
      REAL*8 SOL(NCL + 1), SPRB
      REAL*8 SON(NFG,NCL), SUM1, SUM2, GRFQ(NCL), GRZQ(NCL)
      REAL*8 SINT(NFG,NCL + 1)
      REAL*8 WP(NANG)
      REAL*8 ZLP(NANG), ZINT(NFG,NCL), ZQ(NFG,NCL), DIER

      COMMON /R01/ ALFA, AC, ATMASS, DAF, ATEM
      COMMON /R02/ ABC, AB, AO
      COMMON /R15/ NATE, NINT
      COMMON /R27/ WF
      COMMON /R28/ ZLP, ZINT, ZQ, DIER

      DO 30 J = 1, NG
       DO 20 K = 1, NC
        ZINT(J,K) = 0.0
        DO 10 I = 1, NA
         ZINT(J,K) = ZINT(J,K) + NINT(I,J,K) * WF(I)
   10   CONTINUE
   20  CONTINUE
   30 CONTINUE
      DO 50 K = 1, NC
       AB(K) = 0.0
       DO 40 J = 1, NG
        AB(K) = AB(K) + ABC(J,K) * ZINT(J,K)
   40  CONTINUE
   50 CONTINUE
      RETURN
      END
C
C  ***************************************************************
C  * this subroutine solves the diffusion equation               *
C  ***************************************************************
C

      SUBROUTINE MFDE

      PARAMETER (NANG=24,NFG=64,NCL=151)
      PARAMETER (PI=3.141593)

      REAL*8 A(NCL + 1)
      REAL*8 B(NCL + 1)
      REAL*8 C(NCL + 1)
      REAL*8 R(NCL + 1)

      COMMON /IMT/ J, N
      COMMON /RMT/ A, B, C, R

      LOGICAL TRN, DIFF, LOR, NLOR, SIMRUN, SMTST
      COMMON /L1/ TRN, DIFF, LOR, NLOR, SIMRUN, SMTST

      INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      INTEGER DRT, DIFBC, DIFACC, IIT, TITA
      INTEGER INSB, IRUN, LIN, MEDUSA
      INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      INTEGER USC, WFN, CONV, DBXL, DBXU, NUM
      INTEGER NCP1, NCM1, NAD2
      INTEGER SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

      COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      COMMON /I2/ DRT, DIFBC, DIFACC, IIT, TITA
      COMMON /I3/ INSB, IRUN, LIN, MEDUSA
      COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      COMMON /I7/ USC, WFN, CONV, DBXL, DBXU, NUM
      COMMON /I8/ NCP1, NCM1, NAD2
      COMMON /SMT/ SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

      REAL*8 ALFA(NCL), AC, ATMASS, DAF(NFG,NCL), ATEM(NCL)
      REAL*8 ABC(NFG,NCL), AB(NCL), AO(NFG,NCL)
      REAL*8 BETA(NCL), BO(NFG,NCL)
      REAL*8 CV(NCL), CW, CH(NFG,NCL)
      REAL*8 DL(NCL), DINT(NFG,NCL + 1), PRNTM
      REAL*8 DIIT(NCL), DTIME, DSPR
      REAL*8 ETA(NCL)
      REAL*8 FINT(NFG,NCL + 1), FINL(NFG), FINR(NFG)
      REAL*8 FR(NFG + 1), FQ(NFG,NCL)
      REAL*8 INTR(NANG,NFG,NCL + 1), INT(NANG,NFG,NCL), IZIN(NFG,NCL)
      REAL*8 ITRB, ITER(NFG,NCL)
      REAL*8 NATE(NCL), NINT(NANG,NFG,NCL)
      REAL*8 NPFT(NANG,NFG,NCL), NDIN(NFG,NCL + 1), NZIN(NFG,NCL)
      REAL*8 PMAC(NCL), PINT(NANG,NFG,NCL), PRTIME
      REAL*8 PQIN(NCL + 1), PFG(NCL + 1), PLANK(NFG,NCL)
      REAL*8 PZIN(NFG,NCL + 1), PITR(NFG,NCL), PZIN(NFG,NCL)
      REAL*8 SIGM(NFG,NCL), GRIZ(NCL + 1)
      REAL*8 SOL(NCL + 1), SPRB
      REAL*8 SON(NFG,NCL), SUM1, SUM2, GRFQ(NCL), GRZQ(NCL)
      REAL*8 SINT(NFG,NCL + 1)
      REAL*8 WP(NANG)
      REAL*8 ZLP(NANG), ZINT(NFG,NCL), ZQ(NFG,NCL), DIER

      COMMON /R01/ ALFA, AC, ATMASS, DAF, ATEM
      COMMON /R02/ ABC, AB, AO
```

```
      COMMON /R03/ BETA, BO
      COMMON /R04/ CV, CW, CH
      COMMON /R05/ DL, DINT, PRNTM
      COMMON /R06/ DIST, DTIME, DSPR
      COMMON /R07/ ETA
      COMMON /R071/ FINT, FINL, FINR
      COMMON /R08/ FR, FQ
      COMMON /R11/ INTB, IINT, IZIN
      COMMON /R12/ ITRB, ITER
      COMMON /R13/ NATE, NINT
      COMMON /R16/ NPFT, NDIN, NZIN
      COMMON /R17/ PMAC, PINT, PRTIME
      COMMON /R18/ PGIN, PFGI, PLANK
      COMMON /R181/ PDIN, PITE, PZIN
      COMMON /R21/ SIGM, ORSE
      COMMON /R22/ SOLU, SPRB
      COMMON /R23/ S, SUM1, SUM2, GRFQ, GRZQ
      COMMON /R231/ SINT
      COMMON /R27/ WF
      COMMON /R28/ ZLP, ZINT, ZQ, DIER

      IF (PRES .GE. 3 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1    THEN
       WRITE (8,*)' k iter pstr'
       WRITE (8,10) ((J,K,ITER(J,K),PITE(J,K),K=1,NC),J=1,NG)
  10   FORMAT (1X, I2, 1X, I2, 1X, 1PE10.3, 1X, 1PE10.3)
       END IF
       DO 60 J = 1, NG
        DO 20 K = 1, NCP1
         IF (K .EQ. 1) THEN
          A(K) = 0.0
          B(K) = SUM1 + SIGM(J,K) * BO(J,K) / 4 + 1 / (3 *SIGM(J,K))
          C(K) = SIGM(J,K) * AO(J,K) / 4 - 1 / (3 *SIGM(J,K))
         ELSE IF (K .EQ. NCP1) THEN
          A(K) = SIGM(J,K - 1) * BO(J,K - 1) / 4 - 1 / (3 *SIGM(J,K -
     1    1))
          B(K) = -SUM2 + SIGM(J,K - 1) * AO(J,K - 1) / 4 + 1 / (3 *
     1    SIGM(J,K - 1))
          C(K) = 0.0
         ELSE
          A(K) = SIGM(J,K - 1) * BO(J,K - 1) / 4 - 1 / (3 *SIGM(J,K -
     1    1))
          B(K) = (SIGM(J,K - 1)*AO(J,K - 1) + SIGM(J,K)*BO(J,K)) / 4 +
     1    1 / (3 *SIGM(J,K - 1)) + 1 / (3 *SIGM(J,K))
          C(K) = SIGM(J,K) * AO(J,K) / 4 - 1 / (3 *SIGM(J,K))
         END IF
  20    CONTINUE
        DO 30 K = 1, NCP1
         IF (K .EQ. 1) THEN
          R(K) = SUM1 * PDIN(J,K) + FINT(J,K) + 2 * (SINT(J,K + 1) -
     1    SINT(J,K)) / (3 *SIGM(J,K)) + ZQ(J,K) * DL(K) / 2 - PQ(J,K) *
     2    DL(K) / SIGM(J,K) + ITER(J,K)
         ELSE IF (K .EQ. NCP1) THEN
          R(K) = -SUM2 * PDIN(J,K) - FINT(J,K) - 2 * (SINT(J,K) -
     1    SINT(J,K - 1)) / (3 *SIGM(J,K - 1)) + ZQ(J,K - 1) * DL(K - 1)
     2    / 2 + PQ(J,K - 1) * DL(K - 1) / SIGM(J,K - 1) + ITER(J,K -
     3    1)
         ELSE
          R(K) = ITER(J,K - 1) + ITER(J,K) + SO(J,K - 1)
         END IF
  30    CONTINUE
        IF (PRES .GE. 7 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1     THEN
         WRITE (8,*)'a b c r in group ', J
         WRITE (8,40) (K,A(K),B(K),C(K),R(K),K=1,NCP1)
  40     FORMAT (1X, 'K', I2, 1X, 1PE10.3, 1X, 1PE10.3, 1X, 1PE10.3,
     1       1X, 1PE10.3)
         END IF
         N = NCP1
C  invert the diffusion equation
         CALL LU3
         DO 50 K = 1, NCP1
          NDIN(J,K) = SOLU(K)
  50    CONTINUE
  60   CONTINUE
C**** keep track of the # of times negative diffusion intensity occurs
       DO 80 J = 1, NG
        DO 70 K = 1, NCP1
         IF (NDIN(J,K) .LT. 0) THEN
          NDICNT = NDICNT + 1
         END IF
  70    CONTINUE
  80   CONTINUE
       IF (PRES .GE. 6 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1    THEN
        WRITE (8,*)'dist ndin', TOIT, TIT, OIT, IT, TIT
        WRITE (8,90) ((J,K,DINT(J,K),NDIN(J,K),K=1,NCP1),J=1,NG)
  90    FORMAT (2(1X,'J',I2,1X,'K',I2,3(1PE10.3,1X)))
        END IF
        RETURN
        END
C
C  *********************************************************************
C  * this subroutine computes the spectral radius and determines  *
C  * if diffusion equation                                        *
C  *********************************************************************
C
      SUBROUTINE DIFCONV

      PARAMETER (NANG=24,NFG=64,NCL=151)

      REAL*8 DDIFF, DPDIF, DNDIF
      REAL*8 DSPIN(NCL), DSNIN(NCL)
      REAL*8 TINT

      LO 4CAL TRN, DIFF, LGR, NLGR, SIMRUN, SIMTST

      COMMON /L1/ TRN, DIFF, LGR, NLGR, SIMRUN, SIMTST

      INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      INTEGER DRT, DIFBC, DIFACC, IIT, TITA
      INTEGER INSB, IRUN, LIN, MEDUSA
      INTEGER NA, NG, NC, NF, NDIT, NFFC, NDICNT, NFMUST
      INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      INTEGER TB, TEMEXP, TIT, TOIT, TEMPTD, TIT, TRIN
      INTEGER USC, WFN, CONV, DBXL, DBXU, NUM
      INTEGER NCP1, NCM1, NAD2
      INTEGER SIMTST1, SIMTST2, SIMTST3, SIMTST4, SIMTST5

      COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      COMMON /I2/ DRT, DIFBC, DIFACC, IIT, TITA
      COMMON /I3/ INSB, IRUN, LIN, MEDUSA
      COMMON /I4/ NA, NG, NC, NF, NDIT, NFFC, NDICNT, NFMUST
      COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      COMMON /I6/ TB, TEMEXP, TIT, TOIT, TEMPTD, TIT, TRIN
      COMMON /I7/ USC, WFN, CONV, DBXL, DBXU, NUM
      COMMON /I8/ NCP1, NCM1, NAD2
      COMMON /SMT/ SIMTST1, SIMTST2, SIMTST3, SIMTST4, SIMTST5

      REAL*8 ABC(NFG,NCL), AB(NCL), AO(NFG,NCL)
      REAL*8 DL(NCL), DINT(NFG,NCL + 1), PRNTM
      REAL*8 DIST(NCL), DTIME, DSPR
      REAL*8 FR(NFG + 1), FQ(NFG,NCL)
      REAL*8 NPFT(NANG,NFG,NCL), NDIN(NFG,NCL + 1), NZIN(NFG,NCL)
      REAL*8 WF(NANG)
      REAL*8 ZLP(NANG), ZINT(NFG,NCL), ZQ(NFG,NCL), DIER

      COMMON /R02/ ABC, AB, AO
      COMMON /R05/ DL, DINT, PRNTM
      COMMON /R06/ DIST, DTIME, DSPR
      COMMON /R08/ FR, FQ
      COMMON /R16/ NPFT, NDIN, NZIN
      COMMON /R27/ WF
      COMMON /R28/ ZLP, ZINT, ZQ, DIER

      IF (DRT .LT. 1) THEN
       DO 20 K = 1, NC
        DSNIN(K) = 0.0
        DSPIN(K) = 0.0
        DO 10 J = 1, NG
         DSPIN(K) = DSPIN(K) + ABC(J,K) * DINT(J,K) * (FR(J + 1) -
     1   FR(J))
         DSNIN(K) = DSNIN(K) + ABC(J,K) * NDIN(J,K) * (FR(J + 1) -
     1   FR(J))
  10    CONTINUE
  20   CONTINUE
       DDIFF = 0.0
       DO 30 K = 1, NC
        DDIFF = DDIFF + (((DSNIN(K) - DSPIN(K))/2)**2) * DL(K)
  30   CONTINUE
       DPDIF = SQRT(DDIFF/4)
       DRT = 2
       DO 40 K = 1, NC
        DSPIN(K) = DSNIN(K)
  40   CONTINUE
       GO TO 120
      ELSE
       DO 60 K = 1, NC
        DSNIN(K) = 0.0
        DO 50 J = 1, NG
         DSNIN(K) = DSNIN(K) + ABC(J,K) * NDIN(J,K) * (FR(J + 1) -
     1   FR(J))
  50    CONTINUE
  60   CONTINUE
       DDIFF = 0.0
       DO 70 K = 1, NC
        DDIFF = DDIFF + (((DSNIN(K) - DSPIN(K))/2)**2) * DL(K)
  70   CONTINUE
       DN~IF = SQRT(DDIFF/4)
      END IF
      DSPR = DNDIF / DPDIF
      DPDIF = DNDIF
      IF (PRES .GE. 3 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1    THEN
       WRITE (8,80) DNDIF, DSPR
  80   FORMAT (1X, 'DNT ERR=', 1PE10.3, 5X, 'DIFF SPR=', 1PE10.3)
      END IF
      GO TO 110
      DO 100 J = 1, NG
       DO 90 K = 1, NC
        IF (NDIN(J,K)/DINT(J,K) .GT. 100.0 .OR. NDIN(J,K)/DINT(J,K) .
     1      LE. 0.01) THEN
         SMTST4 = SMTST4 + 1
        END IF
  90   CONTINUE
 100  CONTINUE
      IF (SMTST4 .GT. (NG*NC)*0.05) THEN
       SMTST = .TRUE.
       WRITE (99,*)'inner iteration terminated due to unphysical incres
     1se in ndin'
      END IF
 110  IF (DSPR .GE. 1.00) THEN
       SMTST3 = SMTST3 + 1
       IF (SMTST3 .GE. (NG*NC*0.01)) THEN
        WRITE (99,*)'inner iteration terminated due to dspr being > 1.
     10 too often'
        SMTST = .TRUE.
       END IF
      END IF
 120  DO 130 K = 1, NC
       DSPIN(K) = DSNIN(K)
 130  CONTINUE
      IF (CONVC .EQ. 0) THEN
```

```
      IF (DNDIF .GE. DIER) GO TO 190
     ELSE IF (CONVC .EQ. 1) THEN
      DO 150 J = 1, NO
       DO 140 K = 1, NCP1
        IF (ABS(NDIN(J,K)/DINT(J,K) - 1) .GE. DIER) GO TO 190
  140   CONTINUE
  150  CONTINUE
     ELSE IF (CONVC .EQ. 2) THEN
      DO 180 J = 1, NO
       TINT = 0.0
       DO 160 K = 1, NCP1
        TINT = TINT + NDIN(J,K)
  160   CONTINUE
       DO 170 K = 1, NCP1
        IF (ABS(NDIN(J,K) - DINT(J,K))/TINT) .GE. DIER)
     1    GO TO 190
  170   CONTINUE
  180  CONTINUE
     END IF
     CONV = 0
     RETURN
  190 CONV = 1
     RETURN
     END
C
C  ***************************************************************
C  *  this subroutine solves the diffusion equation using SI     *
C  ***************************************************************
C
      SUBROUTINE DIFFSI

      PARAMETER (NANO=24,NFO=64,NCL=151)

      INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      INTEGER DIRT, DIFBC, DIFACC, IIT, TITA
      INTEGER INSB, IRUN, LIN, MEDUSA
      INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      INTEGER USC, WFN, CONV, DBXL, DBXU, NUM
      INTEGER NCP1, NCM1, NAD2
      INTEGER SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

      COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      COMMON /I2/ DIRT, DIFBC, DIFACC, IIT, TITA
      COMMON /I3/ INSB, IRUN, LIN, MEDUSA
      COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      COMMON /I7/ USC, WFN, CONV, DBXL, DBXU, NUM
      COMMON /I8/ NCP1, NCM1, NAD2
      COMMON /SMT/ SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

      REAL*8 ALFA(NCL), AC, ATMASS, DAF(NFO,NCL), ATEM(NCL)
      REAL*8 ABC(NFO,NCL), AB(NCL), AO(NFO,NCL)
      REAL*8 BETA(NCL), BO(NFO,NCL)
      REAL*8 CV(NCL), CW, CH(NFO,NCL)
      REAL*8 DL(NCL), DINT(NFO,NCL + 1), PRNTM
      REAL*8 DIST(NCL), DTIME, DSPR
      REAL*8 ETA(NCL)
      REAL*8 ITRB, ITER(NFO,NCL)
      REAL*8 NFFT(NANO,NFO,NCL), NDIN(NFO,NCL + 1), NZIN(NFO,NCL)
      REAL*8 ZLP(NANO), ZINT, ZQ, DIER

      COMMON /R01/ ALFA, AC, ATMASS, DAF, ATEM
      COMMON /R02/ ABC, AB, AO
      COMMON /R03/ BETA, BO
      COMMON /R04/ CV, CW, CH
      COMMON /R05/ DL, DINT, PRNTM
      COMMON /R06/ DIST, DTIME, DSPR
      COMMON /R07/ ETA
      COMMON /R12/ ITRB, ITER
      COMMON /R16/ NFFT, NDIN, NZIN
      COMMON /R28/ ZLP, ZINT, ZQ, DIER

      DO 20 K = 1, NC
       AB(K) = 0.0
       DO 10 J = 1, NO
        AB(K) = AB(K) + ABC(J,K) * (AO(J,K)*NDIN(J,K + 1) + BO(J,K)*
     1   NDIN(J,K))
   10  CONTINUE
   20 CONTINUE
      IF (PRES .GE. 4 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1    THEN
       WRITE (8,*)'ab ok0k'
       WRITE (8,30) (K,AB(K),K=1,NC)
   30  FORMAT (1X, 4(1X,I3,1X,E12.1X,1PE10.3,1X))
      END IF
      DO 50 K = 1, NC
       DO 40 J = 1, NO
        ITER(J,K) = DL(K) * CH(J,K) * ETA(K) * AB(K) / 4
   40  CONTINUE
   50 CONTINUE
      IF (DIFACC .EQ. 1 .AND. IIT .GE. 2) THEN
       DO 70 K = 1, NC
        DO 60 J = 1, NO
         DAF(J,K) = (AO(J,K)*NDIN(J,K + 1) + BO(J,K)*NDIN(J,K)) / (
     1    AO(J,K)*DINT(J,K + 1) + BO(J,K)*DINT(J,K))
   60   CONTINUE
   70  CONTINUE
       DO 90 K = 1, NC
        DO 80 J = 1, NO
         ITER(J,K) = ITER(J,K) * DAF(J,K)
   80   CONTINUE
   90  CONTINUE
      END IF
```

```
      RETURN
      END
C
C  ***************************************************************
C  *    this subroutine computes temperature in each cell        *
C  ***************************************************************
C
      SUBROUTINE TEMPER

      PARAMETER (NANO=24,NFO=64,NCL=151)
      PARAMETER (BK=7.560667E-16,PK=6.6261E-34)
      PARAMETER (BK=1.3807E-23,XP=3.0E08,EVE=1.6022E-19)
      PARAMETER (TCF=EVE/BK,OK=8.5144,PI=3.141593,AO=PK/(BK*TCF))

      REAL*8 NERED(NCL)

      INTEGER INSB, IRUN, LIN, MEDUSA
      INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      INTEGER USC, WFN, CONV, DBXL, DBXU, NUM

      COMMON /I3/ INSB, IRUN, LIN, MEDUSA
      COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
      COMMON /I7/ USC, WFN, CONV, DBXL, DBXU, NUM

      REAL*8 ABC(NFO,NCL), AB(NCL), AO(NFO,NCL)
      REAL*8 BETA(NCL), BO(NFO,NCL)
      REAL*8 DIST(NCL), DTIME, DSPR
      REAL*8 ETA(NCL)
      REAL*8 INLB(NFO), INRB(NFO), ITSL, IERED(NCL), IERR
      REAL*8 NATE(NCL), NINT(NANO,NFO,NCL)
      REAL*8 PMAC(NCL), PINT(NANO,NFO,NCL), PRTIME
      REAL*8 TTIME, TOU, TERR, TELB

      COMMON /R02/ ABC, AB, AO
      COMMON /R03/ BETA, BO
      COMMON /R06/ DIST, DTIME, DSPR
      COMMON /R07/ ETA
      COMMON /R10/ INLB, INRB, ITSL, IERED, IERR
      COMMON /R15/ NATE, NINT
      COMMON /R17/ PMAC, PINT, PRTIME
      COMMON /R24/ TTIME, TOU, TERR, TELB

      DO 10 K = 1, NC
       NERED(K) = (ETA(K)/(EP**PMAC(K))) * (1.0**1*AB(K) + IERED(K)*(
     1  DTIME**BETA(K)))
       NATE(K) = ((NERED(K)/BK)**0.25)
   10 CONTINUE
      IF (MEDUSA .EQ. 0) THEN
       DO 20 K = 1, NC
        NATE(K) = NATE(K) / TCF
   20  CONTINUE
       IF (PRES .GE. 1 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1     THEN
        WRITE (6,30) TTIME, TOIT, TIIT, TIT
   30   FORMAT (1X, 'temp is:', 1PE10.3, 5X, 'toit tiit tit=',
     1       3(1X,I3))
        WRITE (6,40) (DIST(K),NATE(K),K=1,NC)
   40   FORMAT (3(1PE10.3,1X,1PE10.3,1X))
       END IF
      END IF
      RETURN
      END
C
C  ***************************************************************
C  *    determine if temperature is converged                    *
C  ***************************************************************
C
      SUBROUTINE TEMCON

      PARAMETER (NANO=24,NFO=64,NCL=151)

      INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN

      COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN

      REAL*8 ALFA(NCL), AC, ATMASS, DAF(NFO,NCL), ATEM(NCL)
      REAL*8 DIST(NCL), DTIME, DSPR
      REAL*8 NATE(NCL), NINT(NANO,NFO,NCL)
      REAL*8 TTIME, TOU, TERR, TELB

      COMMON /R01/ ALFA, AC, ATMASS, DAF, ATEM
      COMMON /R06/ DIST, DTIME, DSPR
      COMMON /R15/ NATE, NINT
      COMMON /R24/ TTIME, TOU, TERR, TELB

      LOGICAL TRN, DIFF, LOR, NLOR, SIMRUN, SMTST
      COMMON /L1/ TRN, DIFF, LOR, NLOR, SIMRUN, SMTST

      IF (TCONT .EQ. 0) THEN
       GO TO 30
      END IF
      DO 10 K = 1, NC
       IF (ABS(NATE(K)/ATEM(K) - 1) .GT. TERR) THEN
        CONT = 1
        GO TO 30
       END IF
   10 CONTINUE
      CONT = 0
```

```
      IF ( .NOT. SIMRUN) THEN
       DO 20 K = 1, NC
        IF (ABS(NATE0(K)/ATEM(K) - 1) .GT. 0.01) THEN
         GO TO >0
        END IF
   20   CONTINUE
        DTIME = 2 * DTIME
       END IF
       30 DO 40 K = 1, NC
        ATEM(K) = NATE(K)
       40 CONTINUE
       RETURN
       END

C**** f1 function is used for computing planckian absorption coefficient
C**** and initial intensity (which is assumed to be planckian)

       FUNCTION FPLNK(X)

       REAL*8 X, FPLNK

       INTRINSIC EXP

       IF (ABS(X) .LT. 1.E-06) THEN
        FPLNK = X * X
       ELSE
        FPLNK = (X**3) / (EXP(X) - 1.0)
       END IF
       RETURN
       END

C**** f2 and f3 functions are used for computing rosseland absorp
C**** ion coefficient

       FUNCTION F2(X)
       REAL*8 X, F2
       INTRINSIC EXP
       IF (ABS(X) .LT. 1.E-6) THEN
        F2 = X * X * EXP(X)
       ELSE
        F2 = ((X**4)*EXP(X)) / ((EXP(X) - 1.0)**2)
       END IF
       RETURN
       END
C
       FUNCTION F3(X)
       REAL*8 X, F3
       INTRINSIC DEXP
       IF (ABS(X) .LT. 1.E-6) THEN
        F3 = X ** 4 * EXP(2.*X)
       ELSE
        F3 = ((X**7)*EXP(2.*X)) / ((EXP(X) - 1.0)**3)
       END IF
       RETURN
       END
C
       FUNCTION FSIG(X)

       REAL*8 X, FSIG

       INTRINSIC EXP

       IF (ABS(X) .LT. 1.E-06) THEN
        FSIG = -1 / X ** 2
       ELSE
        FSIG = (1 - EXP(-X)) / X ** 3
       END IF
       RETURN
       END
C
C ***********************************************************************
C *    following subroutine computes the integral of a given func-     *
C * ction using romberg method.                                        *
C ***********************************************************************
C
       SUBROUTINE ROMINT( D, E, RES)

       REAL*8 D, DEL, DIFF
       REAL*8 ERR
       REAL*8 E, F
       REAL*8 RES
       REAL*8 X, Z(30,30)

       EXTERNAL F

       IF (D .EQ. 0) THEN
        D = 1.0E-06
       END IF
       ERR = 1.0E-06 * ((D/E)**4)
       I = 1
       DEL = E - D
       Z(1,1) = 0.5 * DEL * (F(D) + F(E))
      10 J = 2 ** (I - 1)
       DEL = DEL / 2
       I = I + 1
       Z(I,1) = 0.5 * Z(I - 1,1)
       DO 20 K = 1, J
        X = D + ((2.*K) - 1) * DEL
        Z(I,1) = Z(I,1) + DEL * F(X)
      20 CONTINUE
       DO 30 K = 2, I
        Z(I,K) = (4.**(K - 1)*Z(I,K - 1) - Z(I - 1,K - 1)) / (4.**(K -
     1  1) - 1.)
      30 CONTINUE
       DIFF = ABS(Z(I,J) - Z(I,J - 1))
       IF (DIFF .LT. ERR) GO TO 40
       IF (I .LT. 20) GO TO 10
       WRITE (6,*)'required precision could not be achieved'
       STOP
      40 RES = Z(I,J)
       RETURN
       END
C
C ***********************************************************************
C  * this subroutine inverts the tridiagonal matrix by LU       *
C  * decomposition                                              *
C ***********************************************************************
C
       SUBROUTINE LU3

       PARAMETER (NANO=24,NFG=64,NCL=151)

       LOGICAL TRN, DIFF, LOR, NLOR, SIMRUN, SMTST
       COMMON /L1/ TRN, DIFF, LOR, NLOR, SIMRUN, SMTST

       INTEGER DRT, DIFBC, DIFACC, IIT, TITA
       INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
       INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
       INTEGER TB, TEMEXP, TIT, TOIT, TEMPTD, TIT, TRIN
       INTEGER UBC, WFN, CONV, DBXL, DBXU, NUM
       INTEGER NCP1, NCM1, NAD2
       INTEGER SMTST1, SMTST2, SMTST3, SMTST4, SMTST5

       COMMON /I2/ DRT, DIFBC, DIFACC, IIT, TITA
       COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
       COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
       COMMON /I6/ TB, TEMEXP, TIT, TOIT, TEMPTD, TIT, TRIN
       COMMON /I7/ UBC, WFN, CONV, DBXL, DBXU, NUM
       COMMON /I8/ NCP1, NCM1, NAD2
       COMMON /SMT/ SMTST1, SMTST2, SMTST3, SMTST4, SMTST5
       COMMON /RMT/ A, B, C, R

       REAL*8 DL(NCL), DINT(NFG,NCL + 1), PRNTM
       COMMON /R05/ DL, DINT, PRNTM

       REAL*8 A(NCL + 1), B(NCL + 1), C(NCL + 1), R(NCL + 1)
       REAL*8 SOLU(NCL + 1), SPRB
       REAL*8 OA(NCL + 1), OB(NCL + 1), OC(NCL + 1)
       REAL*8 OR(NCL + 1)
       REAL*8 NR(NCL + 1), ERR(NCL + 1)
       REAL*8 GAM(NCL + 1), BET

       COMMON /R22/ SOLU, SPRB

       COMMON /IMT/ I, N

       IF (PRES .GE. 6 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1     THEN
        WRITE (8,*)'values in lu of group ', J
        WRITE (8,*)'a b c r'
        WRITE (8,10) (K,A(K),B(K),C(K),R(K),K=1,N)
       10  FORMAT (1X, 'K', I2, 1X, 1PE11.4, 1X, 1PE11.4, 1X, 1PE11.4, 1X,
     1       1PE11.4)
       END IF

       DO 20 K = 1, N
        OA(K) = A(K)
        OC(K) = C(K)
        OB(K) = B(K)
        OR(K) = R(K)
       20 CONTINUE
       IF (B(1) .EQ. 0.0) THEN
        WRITE (8,*)'SOLVE SOLU(2) BY ELIMINATION, LEAVING N-1 EQUATION'
        PAUSE
       END IF
       BET = B(1)
       SOLU(1) = R(1) / BET
       DO 30 K = 2, N
        GAM(K) = C(K - 1) / BET
        BET = B(K) - A(K) * GAM(K)
        SOLU(K) = (R(K) - A(K)*SOLU(K - 1)) / BET
       30 CONTINUE
       DO 40 K = N - 1, 1, -1
        SOLU(K) = SOLU(K) - GAM(K + 1) * SOLU(K + 1)
       40 CONTINUE
       DO 50 K = 1, N
        IF (K .EQ. 1) THEN
         NR(K) = OB(K) * SOLU(K) + OC(K) * SOLU(K + 1)
        ELSE IF (K .EQ. N) THEN
         NR(K) = OA(K) * SOLU(K - 1) + OB(K) * SOLU(K)
        ELSE
         NR(K) = OA(K) * SOLU(K - 1) + OB(K) * SOLU(K) + OC(K) * SOLU(
     1   K + 1)
        END IF
        IF (NR(K) .EQ. 0) THEN
         ERR(K) = -999.9999
        ELSE
         ERR(K) = 1 - OR(K) / NR(K)
        END IF
       50 CONTINUE
       DO 60 K = 1, N
        IF (ABS(ERR(K)) .GT. 0.01) GO TO 70
       60 CONTINUE
       RETURN
       70 IF (NPR .EQ. 0) THEN
          WRITE (6,*)'soln is ill balanced for group', J, TOIT, IIT, TIT
          WRITE (6,80) (K,A(K),B(K),C(K),R(K),K=1,N)
       80  FORMAT (1X, I2, 1X, 'a=', 1PE10.3, 1X, 'b=', 1PE10.3, 1X, 'c=',
     1       1PE10.3, 1X, 'r=', 1PE10.3)
          WRITE (6,90) (K,OR(K),NR(K),SOLU(K),DINT(J,K),K=1,N)
       90  FORMAT (1X, I2, 'or=', 1PE10.3, 1X, 'nr=', 1PE10.3, 1X, 'solu=',
     1       1PE10.3, 1X, 'dint=', 1PE10.3)
```

```
      SMTST2 = SMTST2 + 1
      IF (SMTST2 .GT. INT((NG*NC)*.05)) THEN
       WRITE (6,*)'program terminated in LU entst2'
       SMTST = .TRUE.
      END IF
      WRITE (6,*)'enter 1 if above message to be removed'
      READ (5,*) NPR
     END IF
     RETURN
     END
C
C ***************************************************************
C *    following subroutine provides zeroes and weight functions  *
C * of Legendre Polynomial                                      *
C ***************************************************************
C
C
     SUBROUTINE LPL
C
     PARAMETER (NANO=24,NFO=64,NCL=131)
C
     INTEGER NA, NG, NC, NF, NDIT, NFFC, NDICNT, NFMUST
     INTEGER NCP1, NCM1, NAD2
     COMMON /II/ NCP1, NCM1, NAD2
C
     REAL*8 B(NFO,NCL), SUM1, SUM2, GRFQ(NCL), GRZQ(NCL)
     REAL*4 WP(NANO)
     REAL*8 ZLP(NANO), ZINT(NFO,NCL), ZQ(NFO,NCL), DIER
C
     COMMON /I4/ NA, NG, NC, NF, NDIT, NFFC, NDICNT, NFMUST
C
     COMMON /R23/ S, SUM1, SUM2, GRFQ, GRZQ
     COMMON /R27/ WP
     COMMON /R28/ ZLP, ZINT, ZQ, DIER
C
     IF (NA .EQ. 2) THEN
      WP(1) = 1.000000
      ZLP(1) = 0.577353
     ELSE IF (NA .EQ. 4) THEN
      WP(1) = 0.652142
      WP(2) = 0.347858
      ZLP(1) = 0.339981
      ZLP(2) = 0.861136
     ELSE IF (NA .EQ. 6) THEN
      WP(1) = 0.467914
      WP(2) = 0.360762
      WP(3) = 0.171325
      ZLP(1) = 0.238619
      ZLP(2) = 0.661209
      ZLP(3) = 0.932470
     ELSE IF (NA .EQ. 8) THEN
      WP(1) = 0.362684
      WP(2) = 0.313707
      WP(3) = 0.222381
      WP(4) = 0.101229
      ZLP(1) = 0.183435
      ZLP(2) = 0.525532
      ZLP(3) = 0.796667
      ZLP(4) = 0.960290
     ELSE IF (NA .EQ. 10) THEN
      WP(1) = 0.295524
      WP(2) = 0.269267
      WP(3) = 0.219086
      WP(4) = 0.149451
      WP(5) = 0.066671
      ZLP(1) = 0.148874
      ZLP(2) = 0.433395
      ZLP(3) = 0.679410
      ZLP(4) = 0.865063
      ZLP(5) = 0.973907
     ELSE IF (NA .EQ. 12) THEN
      WP(1) = 0.249147
      WP(2) = 0.233493
      WP(3) = 0.203167
      WP(4) = 0.160078
      WP(5) = 0.106939
      WP(6) = 0.047175
      ZLP(1) = 0.125233
      ZLP(2) = 0.367832
      ZLP(3) = 0.587318
      ZLP(4) = 0.769905
      ZLP(5) = 0.904117
      ZLP(6) = 0.981561
     ELSE IF (NA .EQ. 16) THEN
      WP(1) = 0.189451
      WP(2) = 0.182603
      WP(3) = 0.169157
      WP(4) = 0.149596
      WP(5) = 0.124628
      WP(6) = 0.095159
      WP(7) = 0.062254
      WP(8) = 0.027152
      ZLP(1) = 0.095013
      ZLP(2) = 0.281604
      ZLP(3) = 0.458017
      ZLP(4) = 0.617876
      ZLP(5) = 0.755404
      ZLP(6) = 0.865631
      ZLP(7) = 0.944575
      ZLP(8) = 0.989401
     ELSE IF (NA .EQ. 20) THEN
      WP(1) = 0.152753
      WP(2) = 0.149173
      WP(3) = 0.142096
      WP(4) = 0.131689
      WP(5) = 0.118195
      WP(6) = 0.101930
```



```
      WP(7) = 0.083277
      WP(8) = 0.062672
      WP(9) = 0.040601
      WP(10) = 0.017614
      ZLP(1) = 0.076527
      ZLP(2) = 0.227786
      ZLP(3) = 0.373706
      ZLP(4) = 0.510867
      ZLP(5) = 0.636054
      ZLP(6) = 0.746332
      ZLP(7) = 0.839117
      ZLP(8) = 0.912234
      ZLP(9) = 0.963972
      ZLP(10) = 0.993129
     ELSE IF (NA .EQ. 24) THEN
      WP(1) = 0.127938
      WP(2) = 0.125837
      WP(3) = 0.121670
      WP(4) = 0.115506
      WP(5) = 0.107444
      WP(6) = 0.097619
      WP(7) = 0.086190
      WP(8) = 0.073346
      WP(10) = 0.044277
      WP(11) = 0.028531
      WP(12) = 0.012341
      ZLP(1) = 0.064057
      ZLP(2) = 0.191119
      ZLP(3) = 0.315043
      ZLP(4) = 0.433794
      ZLP(5) = 0.545421
      ZLP(6) = 0.648909
      ZLP(7) = 0.740124
      ZLP(8) = 0.886416
      ZLP(10) = 0.934273
      ZLP(11) = 0.974729
      ZLP(12) = 0.995187
     ELSE
      WRITE (6,10)
 10   FORMAT (1X, 'NA CAN NOT BE EQUAL TO ODD # OR 14,18 OR 22, CHANGE
     1 THE VALUE FOR NA')
      STOP
     END IF
     DO 20 I = 1, NAD2
      WP(NA + 1 - I) = WP(I)
      ZLP(NA + 1 - I) = -ZLP(I)
 20  CONTINUE
     SUM1 = 0.0
     SUM2 = 0.0
     DO 30 I = 1, NAD2
      SUM1 = SUM1 + ZLP(I) * WP(I)
 30  CONTINUE
     DO 40 I = NAD2 + 1, NA
      SUM2 = SUM2 + ZLP(I) * WP(I)
 40  CONTINUE
     RETURN
     END
C
C ***************************************************************
C *  this subroutine runs this code for the model problem for   *
C *  cases.                                                     *
C ***************************************************************
C
     SUBROUTINE RUNTST(IT)
C
     PARAMETER (NANO=24,NFO=64,NCL=131)
C
     INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
     INTEGER DRT, DIFBC, DIFACC, IT, TITA
     INTEGER INSB, IRUN, LIN, MEDUSA
     INTEGER OIT, OITA, PRES, RT, SETBOU, SCR, TRNACC
C
     COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
     COMMON /I2/ DRT, DIFBC, DIFACC, IT, TITA
     COMMON /I3/ INSB, IRUN, LIN, MEDUSA
     COMMON /I5/ OIT, OITA, PRES, RT, SETBOU, SCR, TRNACC
C
     LOGICAL TRN, DIFF, LGR, NLGR, SIMRUN, SMTST
     COMMON /L1/ TRN, DIFF, LGR, NLGR, SIMRUN, SMTST
C
     INTEGER NDIS(8), IT
     REAL*8 TME2(16)
     REAL*4 MAXT
     REAL*8 TTIME, TOU, TERR, TELB
     REAL*8 DIST(NCL), DTIME, DIFR
C
     COMMON /R14/ MAXT
     COMMON /R24/ TTIME, TOU, TERR, TELB
     COMMON /R66/ DIST, DTIME, DIFR
C
     IF (IT .EQ. 0) THEN
      NDIS(1) = 2
      NDIS(2) = 5
      NDIS(3) = 10
      NDIS(4) = 20
      NDIS(5) = 50
      NDIS(6) = 100
      NDIS(7) = 500
      NDIS(8) = 1000
      TME2(1) = 1.00E-12
      TME2(2) = 2.00E-12
      TME2(3) = 5.00E-12
      TME2(4) = 1.00E-11
      TME2(5) = 2.00E-11
      TME2(6) = 5.00E-11
      TME2(7) = 1.00E-10
```

```
      TME2(8) = 2.00E-10
      TME2(9) = 5.00E-10
      TME2(10) = 1.00E-09
      TME2(11) = 2.00E-09
      TME2(12) = 5.00E-09
      TME2(13) = 1.00E-08
      TME2(14) = 2.00E-08
      TME2(15) = 5.00E-08
      TME2(16) = 2.00E-07
      K = 0
     END IF
     WRITE (8,*)'ire dt =', TRN, DB, IT + 1
     IF ( .NOT. TRN) THEN
      IT = IT + 1
      DTIME = TME2(IT)
      TTIME = DTIME
      TRN = .TRUE.
      DB = NDB(1)
      IF (TTIME .GE. MAXT) THEN
       WRITE (6,*)'analysis is complete'
       STOP
      ELSE
       RETURN
      END IF
     END IF
  10 IF ( .NOT. DIFF) THEN
      TRNACC = 1
      DIFACC = 0
      IF (DB .GT. 500) THEN
       K = 0
       DIFF = .TRUE.
       DIFACC = 2
       DB = NDB(1)
       LIN = 0
       GO TO 10
      ELSE
       K = K + 1
       DB = NDB(K)
       RETURN
      END IF
     ELSE IF ( .NOT. LOR) THEN
      IF (DB .GT. 500) THEN
       K = 0
       LOR = .TRUE.
       DB = NDB(1)
       LIN = 1
       GO TO 10
      ELSE
       K = K + 1
       DB = NDB(K)
       RETURN
      END IF
      WRITE (8,*)'reign dir', DIFF, DB
     ELSE IF ( .NOT. NLOR) THEN
      IF (DB .GT. 500) THEN
       K = 0
       NLOR = .TRUE.
       DB = NDB(1)
       GO TO 10
      ELSE
       K = K + 1
       DB = NDB(K)
       RETURN
      END IF
     ELSE
      WRITE (8,*)'ire diff lgr reign dir', TRN, DIFF, LOR, NLOR, SIMRUN,
     1     DB
      TRN = .FALSE.
      DIFF = .FALSE.
      LOR = .FALSE.
      NLOR = .FALSE.
      DB = NDB(1)
      GO TO 10
     END IF
     END
C    ************************************************************************
C    *  this subroutine solves the grey equation                            *
C    ************************************************************************
C
      SUBROUTINE GRIDE

      PARAMETER (NANO=24,NPO=64,NCL=131)
      PARAMETER (PI=3.141593)

      LOGICAL TRN, DIFF, LOR, NLOR, SIMRUN, SMTST
      COMMON /L1/ TRN, DIFF, LOR, NLOR, SIMRUN, SMTST

      INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      INTEGER DRT, DIFBC, DIFACC, IT, TITA
      INTEGER INSR, IRUN, LIN, MEDUSA
      INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      INTEGER TB, TEMEXP, TIT, TOIT, TEMPTD, TIT, TRIN
      INTEGER UBC, WFN, CONV, DBXL, DBXU, NUM
      INTEGER NCP1, NCM1, NAD2

      COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
      COMMON /I2/ DRT, DIFBC, DIFACC, IT, TITA
      COMMON /I3/ INSR, IRUN, LIN, MEDUSA
      COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
      COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
      COMMON /I6/ TB, TEMEXP, TIT, TOIT, TEMPTD, TIT, TRIN
      COMMON /I7/ UBC, WFN, CONV, DBXL, DBXU, NUM
      COMMON /I8/ NCP1, NCM1, NAD2
```



```
      REAL*8 SUMTH(NCL), SUMPH(NCL)

      REAL*8 AAO(NCL), A(NCL + 1)
      REAL*8 BBO(NCL), B(NCL + 1)
      REAL*8 CONCL + 1)
      REAL*8 DUMF(NCL)
      REAL*8 FUNA(NCL), FUNC(NCL), FUND(NCL), FUNE(NCL)
      REAL*8 FUNF(NFG,NCL), FUNG(NFG,NCL), FUNH(NCL)
      REAL*8 GINT(NCL + 1), GRF(NCL + 1)
      REAL*8 ITRB, ITER(NFG,NCL)
      REAL*8 SGIN(NCL + 1)
      REAL*8 NPPT(NANG,NFG,NCL), NDIN(NFG,NCL + 1), NZIN(NFG,NCL)
      REAL*8 PHI(NFG,NCL)
      REAL*8 R(NCL + 1)
      REAL*8 GRS(NCL), SDD(NCL), SUMZ(NCL), SL, SR
      REAL*8 THETA(NFG,NCL)
      REAL*8 ZETA(NFG,NCL)

      COMMON /IMT/ I, N
      COMMON /RM7/ A, B, C, R

      REAL*8 ALFA(NCL), AC, ATMASS, DAF(NFG,NCL), ATEM(NCL)
      REAL*8 ABC(NFG,NCL), AB(NCL), AO(NFG,NCL)
      REAL*8 BETA(NCL), BO(NFG,NCL)
      REAL*8 CV(NCL), CW, CH(NFG,NCL)
      REAL*8 DL(NCL), DINT(NFG,NCL + 1), PRNTM
      REAL*8 ETA(NCL)
      REAL*8 FR(NFG + 1), FQ(NFG,NCL)
      REAL*8 FINT(NFG,NCL + 1), FINL(NFG), FINR(NFG)
      REAL*8 INTR(NANG,NFG,NCL + 1), IINT(NANG,NFG,NCL), IZIN(NFG,NCL)
      REAL*8 PGIN(NCL + 1), PFGR(NCL + 1), PLANK(NFG,NCL)
      REAL*8 PDIN(NFG,NCL + 1), PITE(NFG,NCL), PZIN(NFG,NCL)
      REAL*8 PAB(NCL)
      REAL*8 SIGM(NFG,NCL), GRSI(NCL + 1)
      REAL*8 SOLU(NCL + 1), SPRB
      REAL*8 SO(NFG,NCL), SUM1, SUM2, GRFQ(NCL), GRZQ(NCL)
      REAL*8 SINT(NFG,NCL + 1)
      REAL*8 TTIME, TOU, TERR, TELB
      REAL*8 ZLP(NANG), ZINT(NFG,NCL), ZQ(NFG,NCL), DIER

      COMMON /R01/ ALFA, AC, ATMASS, DAF, ATEM
      COMMON /R02/ ABC, AB, AO
      COMMON /R03/ BETA, BO
      COMMON /R04/ CV, CW, CH
      COMMON /R05/ DL, DINT, PRNTM
      COMMON /R07/ ETA
      COMMON /R071/ FINT, FINL, FINR
      COMMON /R08/ FR, FQ
      COMMON /R11/ INTR, IINT, IZIN
      COMMON /R12/ ITRB, ITER
      COMMON /R14/ NPPT, NDIN, NZIN
      COMMON /R16/ PGIN, PFGR, PLANK
      COMMON /R161/ PDIN, PITE, PZIN
      COMMON /R162/ PAB
      COMMON /R21/ SIGM, GRSI
      COMMON /R22/ SOLU, SPRB
      COMMON /R23/ S, SUM1, SUM2, GRFQ, GRZQ
      COMMON /R231/ SINT
      COMMON /R24/ TTIME, TOU, TERR, TELB
      COMMON /R28/ ZLP, ZINT, ZQ, DIER

      DO 20 K = 1, NCP1
       GINT(K) = 0.0
       DO 10 J = 1, NG
        GINT(K) = GINT(K) + NDIN(J,K)
   10  CONTINUE
   20 CONTINUE
      DO 40 K = 1, NC
       AAO(K) = 0.0
       BBO(K) = 0.0
       DO 30 J = 1, NG
        AAO(K) = AAO(K) + AO(J,K) * NDIN(J,K + 1)
        BBO(K) = BBO(K) + BO(J,K) * NDIN(J,K)
   30  CONTINUE
       AAO(K) = AAO(K) / GINT(K + 1)
       BBO(K) = BBO(K) / GINT(K)
   40 CONTINUE
      IF (PRES .GE. 3 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1    THEN
       WRITE (8,*)'into bloc'
       WRITE (8,50) (K,AAO(K),BBO(K),K=1,NC)
   50  FORMAT (1X, 2(I5,2(1X,E12.3)))
      END IF
      DO 70 K = 1, NCM1
       GRS(K) = 0.0
       DO 60 J = 1, NG
        GRS(K) = GRS(K) + SG(J,K)
   60  CONTINUE
   70 CONTINUE
      DO 90 K = 1, NC
       DO 80 J = 1, NG
        ZETA(J,K) = (1 + ALFA(K)*ABC(J,K)*ETA(K)) * TOU * DL(K)
        FUNF(J,K) = AO(J,K) * NDIN(J,K + 1) + BO(J,K) * NDIN(J,K)
   80  CONTINUE
   90 CONTINUE
      IF (PRES .GE. 4 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
     1    THEN
       WRITE (8,*)'ire'
       WRITE (8,100) (K,GRS(K),K=1,NCM1)
  100  FORMAT (1X, 4(I5,E12.3))
       WRITE (8,*)'zeta finf'
       WRITE (8,110) ((J,K,ZETA(J,K),FUNF(J,K),K=1,NC),J=1,NG)
  110  FORMAT (1X, 2(I5,E12.3,1X,I5,2(1PE10.3,1X)))
      END IF
      DO 130 K = 1, NC
```

```
          FUNH(IC) = 0.0
          DO 120 J = 1, NG
           FUNH(IC) = FUNH(IC) + ABC(J,IC) * (AAO(IC)*GINT(IC + 1) + BBO(IC)*
     1    GINT(IC))
  120   CONTINUE
  130 CONTINUE
      SL = PGIN(1) * SUM1 + DL(1) * GRZQ(1) / 2 - DL(1) * GRFQ(1) + 2 *
     1GRSK(1) / 3 + PFGR(1)
      SR = PGIN(NCP1) * SUM2 - DL(NC) * GRZQ(NC) / 2 - DL(NC) * GRFQ(NC)
     1 + 2 * GRSK(NC) / 3 + PFGR(NCP1)
      IF (LIN .EQ. 0) THEN
C**** use the linear grey model for accelerating the diffusion
C**** equation
        DO 150 K = 1, NC
         DUMF(K) = 0.0
         DO 140 J = 1, NG
          DUMF(K) = DUMF(K) + CHI(J,K) / (ABC(J,K) + TOU)
  140    CONTINUE
  150   CONTINUE
        DO 170 K = 1, NC
         DO 160 J = 1, NG
          THETA(J,K) = CHI(J,K) / ((ABC(J,K) + TOU)*DUMF(K))
          PHI(J,K) = THETA(J,K)
  160    CONTINUE
  170   CONTINUE
        DO 190 K = 1, NC
         FUNA(K) = 0.0
         SUMZ(K) = 0.0
         DO 180 J = 1, NG
          FUNA(K) = FUNA(K) + PHI(J,K) / SIGMA(J,K)
          SUMZ(K) = SUMZ(K) + ZETA(J,K) * THETA(J,K)
  180    CONTINUE
  190   CONTINUE
        DO 210 K = 1, NC
         SDD4(K) = 0.0
         FUNC(K) = 0.0
         DO 200 J = 1, NG
          SDD4(K) = SDD4(K) + (NDIN(J,K + 1) - NDIN(J,K)) / SIGMA(J,K)
          FUNC(K) = FUNC(K) + ZETA(J,K) * FUNF(J,K)
  200    CONTINUE
         FUND(K) = FUNA(K) * (GINT(K + 1) - GINT(K))
         FUNE(K) = SUMZ(K) * (AAO(K)*GINT(K + 1) + BBO(K)*GINT(K))
  210   CONTINUE
        DO 220 K = 1, NCP1
         IF (K .EQ. 1) THEN
          IF (DIFBC .EQ. 0) THEN
           R(K) = SUM1 * PGIN(K) + PFGR(K) + SDD4(K) / 3 - FUND(K) /
     1     3 + DL(K) * GRZQ(K) / 2 - DL(K) * GRFQ(K) + 2 * GRSK(K) /
     2     3 - FUNC(K) / 4 + FUNE(K) / 4
          ELSE IF (DIFBC .EQ. 1) THEN
           R(K) = SUM1 * (PGIN(K) - GINT(K)) + PFGR(K) + SDD4(K) / 3
     1     - FUND(K) / 3 + DL(K) * GRZQ(K) / 2 - DL(K) * GRFQ(K) + 2
     2     * GRSK(K) / 3 - FUNC(K) / 4 + FUNE(K) / 4
          ELSE IF (DIFBC .EQ. 2) THEN
           R(K) = ETA(K) * DL(K) * FUNH(K) / 4 + SL
          END IF
         ELSE IF (K .EQ. NCP1) THEN
          IF (DIFBC .EQ. 0) THEN
           R(K) = -SUM2 * PGIN(K) - PFGR(K) - SDD4(K - 1) / 3 + FUND(
     1     K - 1) / 3 - 2 * GRSK(K - 1) / 3 + DL(K - 1) * GRZQ(K - 1)
     2     / 2 + DL(K - 1) * GRFQ(K - 1) - FUNC(K - 1) / 4 + FUNE(K
     3     - 1) / 4
          ELSE IF (DIFBC .EQ. 1) THEN
           R(K) = SUM2 * (GINT(K) - PGIN(K)) - PFGR(K) - SDD4(K - 1)
     1     / 3 + FUND(K - 1) / 3 - 2 * GRSK(K - 1) / 3 + DL(K - 1) *
     2     GRZQ(K - 1) / 2 + DL(K - 1) * GRFQ(K - 1) - FUNC(K - 1) /
     3     4 + FUNE(K - 1) / 4
          ELSE IF (DIFBC .EQ. 2) THEN
           R(K) = -ETA(K - 1) * DL(K - 1) * FUNH(K - 1) / 4 + SR
          END IF
         ELSE
          R(K) = (SDD4(K) - SDD4(K - 1)) / 3 - (FUND(K) - FUND(K - 1))
     1    / 3 - (FUNC(K) + FUNC(K - 1)) / 4 + (FUNE(K) + FUNE(K - 1))
     2    / 4 + GRSK(K - 1)
         END IF
  220   CONTINUE
        ELSE
C**** use the nonlinear grey model for accelerating the diffusion
C**** equation
        DO 240 K = 1, NC
         DO 230 J = 1, NG
          FUNG(J,K) = NDIN(J,K + 1) - NDIN(J,K)
  230    CONTINUE
  240   CONTINUE
        DO 260 J = 1, NG
         DO 250 K = 1, NC
          THETA(J,K) = FUNF(J,K) / (AAO(K)*GINT(K + 1) + BBO(K)*GINT(
     1    K))
          PHI(J,K) = FUNG(J,K) / (GINT(K + 1) - GINT(K))
  250    CONTINUE
  260   CONTINUE
        DO 280 K = 1, NC
         SUMZ(K) = 0.0
         DO 270 J = 1, NG
          SUMZ(K) = SUMZ(K) + ZETA(J,K) * THETA(J,K)
  270    CONTINUE
  280   CONTINUE
        DO 300 K = 1, NC
         FUNA(K) = 0.0
         DO 290 J = 1, NG
          FUNA(K) = FUNA(K) + PHI(J,K) / SIGMA(J,K)
  290    CONTINUE
  300   CONTINUE
        DO 330 K = 1, NCP1
         IF (K .EQ. 1) THEN
          IF (DIFBC .EQ. 0) THEN
```

```
           R(K) = SUM1 * PGIN(K) + PFGR(K) + DL(K) * GRZQ(K) / 2 -
     1     DL(K) * GRFQ(K) + 2 * GRSK(K) / 3
          ELSE IF (DIFBC .EQ. 1) THEN
           R(K) = 0.0
           DO 310 J = 1, NG
            R(K) = R(K) + SUM1 * PDIN(J,K) + FINT(J,K) + 2 * (SINT(
     1      J,K + 1) - SINT(J,K)) / (3 *SIGMA(J,K)) + ZQ(J,K) * DL(K)
     2      / 2 - PQ(J,K) * DL(K) / SIGMA(J,K) + ITER(J,K)
  310      CONTINUE
          ELSE IF (DIFBC .EQ. 2) THEN
           R(K) = ETA(K) * DL(K) * FUNH(K) / 4 + SL
          END IF
         ELSE IF (K .EQ. NCP1) THEN
          IF (DIFBC .EQ. 0) THEN
           R(K) = -SUM2 * PGIN(K) - PFGR(K) + DL(K - 1) * GRZQ(K - 1)
     1     / 2 + DL(K - 1) * GRFQ(K - 1) - 2 * GRSK(K - 1) / 3
          ELSE IF (DIFBC .EQ. 1) THEN
           R(K) = 0.0
           DO 320 J = 1, NG
            R(K) = R(K) - SUM2 * PDIN(J,K) - FINT(J,K) - 2 * (SINT(
     1      J,K) - SINT(J,K - 1)) / (3 *SIGMA(J,K - 1)) + ZQ(J,K - 1)
     2      * DL(K - 1) / 2 + PQ(J,K - 1) * DL(K - 1) / SIGMA(J,K -
     3      1) + ITER(J,K - 1)
  320      CONTINUE
          ELSE IF (DIFBC .EQ. 2) THEN
           R(K) = -ETA(K - 1) * DL(K - 1) * FUNH(K - 1) / 4 + SR
          END IF
         ELSE
          R(K) = GRSK(K - 1)
         END IF
  330   CONTINUE
        END IF
        IF (PRES .GE. 3 .AND. TOIT .GE. DBOL .AND. TOIT .LE. DBOU)
     1  THEN
         DO 350 K = 1, NC
          SUMTH(K) = 0.0
          SUMPH(K) = 0.0
          DO 340 J = 1, NG
           SUMTH(K) = SUMTH(K) + THETA(J,K)
           SUMPH(K) = SUMPH(K) + PHI(J,K)
  340     CONTINUE
  350    CONTINUE
         WRITE (8,*)'dump'
         WRITE (8,360) (K,DUMP(K),K=1,NC)
  360    FORMAT (4(1X,I3,1X,E2.1,1X,1PE10.3))
         WRITE (8,*)'theta phi'
         WRITE (8,370) ((J,K,THETA(J,K),PHI(J,K),K=1,NC),J=1,NG)
  370    FORMAT (2(1X,I3,1X,E2.1,1X,'(',E2.2,1PE10.3,1X,E10.3))
         WRITE (8,*)'zeroth sumphi'
         WRITE (8,380) (K,SUMTH(K),SUMPH(K),K=1,NC)
  380    FORMAT (2(1X,I3,1X,E2.1,1X,2(1PE10.3)))
         WRITE (8,*)'flux sumz'
         WRITE (8,390) (K,FUNA(K),SUMZ(K),K=1,NC)
  390    FORMAT (2(1X,I3,1X,E2.1,1X,2(1PE10.3)))
         WRITE (8,*)'addl func fund func'
         WRITE (8,400) (K,SDD4(K),FUNC(K),FUND(K),FUNE(K),K=1,NC)
  400    FORMAT (1X, I3, 1X, E2.1, 1X, 1PE10.3, 1X, 1PE10.3, 1X, 1PE10.3, 1X,
     1    1PE10.3)
        END IF
        DO 450 K = 1, NCP1
         IF (K .EQ. 1) THEN
          IF (DIFBC .EQ. 0) THEN
           A(K) = 0.0
           B(K) = SUM1 + FUNA(K) / 3 + SUMZ(K) * BBO(K) / 4
           C(K) = -FUNA(K) / 3 + SUMZ(K) * AAO(K) / 4
          ELSE IF (DIFBC .EQ. 1) THEN
           A(K) = 0.0
           B(K) = 0.0
           C(K) = 0.0
           DO 410 J = 1, NG
            B(K) = B(K) + (SIGMA(J,K)*BGO(J,K)/4 + 1/(3*SIGMA(J,K))) *
     1      NDIN(J,K) / GINT(K)
            C(K) = C(K) + (SIGMA(J,K)*AGO(J,K)/4 - 1/(3*SIGMA(J,K))) *
     1      NDIN(J,K) / GINT(K)
  410      CONTINUE
           B(K) = B(K) + SUM1
          ELSE IF (DIFBC .EQ. 2) THEN
           A(K) = 0.0
           B(K) = 0.0
           C(K) = 0.0
           DO 420 J = 1, NG
            B(K) = B(K) + (SIGMA(J,K)*BGO(J,K)/4 + 1/(3*SIGMA(J,K))) *
     1      NDIN(J,K)
            C(K) = C(K) + (SIGMA(J,K)*AGO(J,K)/4 - 1/(3*SIGMA(J,K))) *
     1      NDIN(J,K + 1)
  420      CONTINUE
           B(K) = B(K) / GINT(K) + SUM1
           C(K) = C(K) / GINT(K + 1)
          END IF
         ELSE IF (K .EQ. NCP1) THEN
          IF (DIFBC .EQ. 0) THEN
           A(K) = -FUNA(K - 1) / 3 + SUMZ(K - 1) * BBO(K - 1) / 4
           B(K) = FUNA(K - 1) / 3 + SUMZ(K - 1) * AAO(K - 1) / 4 - SUM2
           C(K) = 0.0
          ELSE IF (DIFBC .EQ. 1) THEN
           A(K) = 0.0
           B(K) = 0.0
           DO 430 J = 1, NG
            A(K) = A(K) + (SIGMA(J,K - 1)*BGO(J,K - 1)/4 - 1/(3*SIGMA(J,
     1      K - 1))) * NDIN(J,K) / GINT(K)
            B(K) = B(K) + (SIGMA(J,K - 1)*AGO(J,K - 1)/4 + 1/(3*SIGMA(J,
     1      K - 1))) * NDIN(J,K) / GINT(K)
  430      CONTINUE
           B(K) = B(K) - SUM2
           C(K) = 0.0
          ELSE IF (DIFBC .EQ. 2) THEN
```

```
3181              A(K) = 0.0
3182              B(K) = 0.0
3183              DO 440 J = 1, NG
3184                A(K) = A(K) - (SIGM(J,K - 1)*BO(J,K - 1)/4 - 1/3*SIGM(J,
3185         1      K - 1))) * NDIN(J,K - 1)
3186                B(K) = B(K) - (SIGM(J,K - 1)*AO(J,K - 1)/4 + 1/3*SIGM(J,
3187         1      K - 1))) * NDIN(J,K)
3188          440   CONTINUE
3189              A(K) = A(K) / GINT(K - 1)
3190              B(K) = B(K) / GINT(K) + SUM2
3191              C(K) = 0.0
3192            END IF
3193            ELSE
3194              A(K) = -FUNA(K - 1) / 3 + SUMZ(K - 1) * BBOO(K - 1) / 4
3195              B(K) = (FUNA(K - 1)) + FUNA(K)) / 3 + (SUMZ(K - 1)*AAO(K - 1)) +
3196         1    SUMZ(K)*BBOO(K)) / 4
3197              C(K) = -FUNA(K) / 3 + SUMZ(K) * AAO(K) / 4
3198            END IF
3199          450 CONTINUE
3200            IF (PRES .GE. 4 .AND. TOIT .GE. DBOL .AND. TOIT .LE. DBOU)
3201           1    THEN
3202            IF (LIN .EQ. 0) THEN
3203              WRITE (8,*)'a b c r in lin grey'
3204            ELSE
3205              WRITE (8,*)'a b c r in nonlin grey'
3206            END IF
3207            WRITE (8,460) (K,A(K),B(K),C(K),R(K),K=1,N)
3208          460   FORMAT (1X, 'K', I2, 1X, 1PE10.3, 1X, 1PE10.3, 1X, 1PE10.3, 1X, 1PE10.3, 1X,
3209           1      1PE10.3)
3210            END IF
3211            N = NCP1
3212            CALL LU3
3213            DO 470 K = 1, NCP1
3214              NGIN(K) = SOLU(K)
3215          470 CONTINUE
3216            IF (PRES .GE. 3 .AND. TOIT .GE. DBOL .AND. TOIT .LE. DBOU)
3217           1    THEN
3218            WRITE (8,*)'gint ngin ngin/gint'
3219            WRITE (8,480) (K,GINT(K),NGIN(K),(NGIN(K)/GINT(K)),K=1,NCP1)
3220          480   FORMAT (1X, 'K', I2, 1X, 1PE10.3, 1X, 1PE10.3, 1X, 1PE10.3)
3221            END IF
3222            IF (PRES .GE. 5 .AND. TOIT .GE. DBOL .AND. TOIT .LE. DBOU)
3223           1    THEN
3224            WRITE (8,490) ((K,J,THETA(J,K)*(AAO(K)*NGIN(K + 1) + BBO(K)*
3225           1  NGIN(K)),THETA(J,K)*(AAO(K)*GINT(K + 1) + BBO(K)*GINT(K)),FUNP(
3226           2  J,K),J=1,NG),K=1,NC)
3227          490   FORMAT (2(1X,'K',I2,1X,'J',I2,1PE10.3,1X,1PE10.3,1X,1PE10.3))
3228            END IF
3229            DO 510 K = 1, NC
3230              AB(K) = 0.0
3231              DO 500 J = 1, NG
3232                AB(K) = AB(K) + ABC(J,K) * (THETA(J,K)*(AAO(K)*NGIN(K + 1) +
3233           1    BBO(K)*NGIN(K)) + FUNP(J,K) - THETA(J,K)*(AAO(K)*GINT(K + 1) +
3234           2    BBO(K)*GINT(K)))
3235          500   CONTINUE
3236          510 CONTINUE
3237            IF (PRES .GE. 3 .AND. TOIT .GE. DBOL .AND. TOIT .LE. DBOU)
3238           1    THEN
3239            WRITE (8,*)'ab grey'
3240            WRITE (8,520) (K,AB(K),K=1,NC)
3241          520   FORMAT (4(1X,'K',I2,1X,1PE10.3))
3242            END IF
3243            DO 540 K = 1, NC
3244              DO 530 J = 1, NG
3245                ITER(J,K) = DL(K) * CH(J,K) * ETA(K) * AB(K) / 4
3246          530   CONTINUE
3247          540 CONTINUE
3248            RETURN
3249            END
3250      C
3251      C     ***************************************************************
3252      C     *  prints time of simulation on a pc with microsoft compiler  *
3253      C     * BUT "C*" comments must be removed before time can be obtained *
3254      C     ***************************************************************
3255      C
3256            SUBROUTINE CPUTM
3257
3258            PARAMETER (NANO=24,NFO=64,NCL=151)
3259
3260            INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
3261            INTEGER DRT, DIFBC, DIFACC, IIT, TITA
3262            INTEGER INSB, IRUN, LIN, MEDUSA
3263            INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
3264            INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
3265            INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
3266
3267            COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
3268            COMMON /I2/ DRT, DIFBC, DIFACC, IIT, TITA
3269            COMMON /I3/ INSB, IRUN, LIN, MEDUSA
3270            COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
3271            COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
3272            COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
3273
3274            REAL*8 NATE(NCL), NINT(NANO,NFO,NCL)
3275            REAL*8 DIST(NCL), DTIME, DSPR
3276            REAL*8 TTIME, TOU, TERR, TELB
3277
3278            COMMON /R06/ DIST, DTIME, DSPR
3279            COMMON /R15/ NATE, NINT
3280            COMMON /R24/ TTIME, TOU, TERR, TELB
3281
3282            LOGICAL TRN, DIFF, LOB, NLOB, SIMRUN, SMTST
3283            COMMON /L1/ TRN, DIFF, LOB, NLOB, SIMRUN, SMTST
3284            REAL*8 STIME, FTIME, RUNTM
3285            COMMON /TM8/ STIME, FTIME, RUNTM
3286
3287            WRITE (99,10) TOIT, TIIT, TIT, OIT, IIT
3288          10 FORMAT (1X, 'TOIT=', I8, 1X, 'TIIT=', I8, 1X, 'TIT=', I4, 1X,
3289           1    'OIT=', I4, 1X, 'IIT=', I3)
3290            WRITE (99,20) (DIST(K),NATE(K),K=1,NC)
3291          20 FORMAT (2(1X,1PE10.3))
3292      C*    CALL GETTIM(IHR, IMIN, ISEC, I100SEC)
3293      C*    FTIME = (IHR*360000 + IMIN*6000 + ISEC*100 + I100SEC)
3294            RUNTM = FTIME - STIME
3295            WRITE (99,40) TRNACC, DIFACC, LIN, DTIME
3296          40 FORMAT (1X, 'trnacc=', I2, 1X, 'difacc=', I2, 1X, 'lin=', I2, 1X,
3297           1    'dtime=', 1PE11.4)
3298            WRITE (99,50) RUNTM / 100
3299            WRITE (6,50) RUNTM / 100
3300          50 FORMAT (1X, 'runtime =', F12.2, ' sec')
3301            IF (RUNTM/100 .GT. 1000.0) THEN
3302              WRITE (99,60) RUNTM / 6000.0
3303          60   FORMAT (1X, 'runtime =', F12.2, 'min')
3304            ELSE IF (RUNTM/100 .GT. 10000.0) THEN
3305              WRITE (99,70) RUNTM / 360000.0
3306          70   FORMAT (1X, 'runtime =', F12.2, ' hrs')
3307            END IF
3308            END
3309      C
3310      C     ***************************************************************
3311      C     *  this subroutine reads the tables and evaluates all the     *
3312      C     *  variables needed for the simulation of this code with MEDSUA *
3313      C     *  this subroutine is equivalent of subroutine model, thisA   *
3314      C     *  over rides any predefined variables, which are redefine here.*
3315      C     ***************************************************************
3316      C
3317            SUBROUTINE TABLES
3318
3319            PARAMETER (NANO=24,NFO=64,NCL=151)
3320            PARAMETER (BK=7.560667E-16,PK=6.6261E-34)
3321            PARAMETER (BK=1.3807E-23,XP=3.0E08,EVB=1.6022E-19)
3322            PARAMETER (TCF=EVE/BK,PI=3.141593,A0=PK/(BK*TCF))
3323
3324            INTEGER ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
3325            INTEGER DRT, DIFBC, DIFACC, IIT, TITA
3326            INTEGER INSB, IRUN, LIN, MEDUSA
3327            INTEGER NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
3328            INTEGER OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
3329            INTEGER TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
3330            INTEGER USC, WPN, CONV, DBOL, DBOU, NUM
3331            INTEGER NCP1, NCM1, NAD2
3332            INTEGER SMTST1, SMTST2, SMTST3, SMTST4, SMTST5
3333            INTEGER MDT, NITT
3334
3335            LOGICAL RTEON
3336
3337            COMMON /I1/ ABVL, AUTACL, CONVC, COUNT, CONT, TCONT, DB, DCOUNT
3338            COMMON /I2/ DRT, DIFBC, DIFACC, IIT, TITA
3339            COMMON /I3/ INSB, IRUN, LIN, MEDUSA
3340            COMMON /I4/ NA, NG, NC, NF, NDIT, NFPC, NDICNT, NFMUST
3341            COMMON /I5/ OIT, OITA, PRES, RT, SETSOU, SCR, TRNACC
3342            COMMON /I6/ TB, TEMEXP, TIIT, TOIT, TEMPTD, TIT, TRIN
3343            COMMON /I7/ USC, WPN, CONV, DBOL, DBOU, NUM
3344            COMMON /I8/ NCP1, NCM1, NAD2
3345            COMMON /SMT/ SMTST1, SMTST2, SMTST3, SMTST4, SMTST5
3346            COMMON /IMD/ MDT, NITT, RTEON
3347
3348            REAL*8 ALFA(NCL), AC, ATMASS, DAF(NFO,NCL), ATEM(NCL)
3349            REAL*8 ABC(NFO,NCL), AB(NCL), AO(NFO,NCL)
3350            REAL*8 BETA(NCL), BO(NFO,NCL)
3351            REAL*8 CV(NCL), CW, CH(NFO,NCL)
3352            REAL*8 DL(NCL), DINT(NFO,NCL + 1), PRNTM
3353            REAL*8 DIST(NCL), DTIME, DSPR
3354            REAL*8 ETA(NCL)
3355            REAL*8 FINT(NFO,NCL + 1), FINL(NFO), FINR(NFO)
3356            REAL*8 FR(NFO + 1), FQ(NFO,NCL)
3357            REAL*8 HELIM
3358            REAL*8 INLB(NFO), INRB(NFO), ITEL, IERED(NCL), IERR
3359            REAL*8 INTB(NANO,NFO,NCL + 1), IINT(NANO,NFO,NCL), IZIN(NFO,NCL)
3360            REAL*8 ITRB, ITER(NFO,NCL)
3361            REAL*8 L, LFL, LOWLIM
3362            REAL*8 MAXT
3363            REAL*8 NATE(NCL), NINT(NANO,NFO,NCL)
3364            REAL*8 NFFT(NANO,NFO,NCL), NDIN(NFO,NCL + 1), NZIN(NFO,NCL)
3365            REAL*8 PMAC(NCL), PINT(NANO,NFO,NCL), PRTIME
3366            REAL*8 PQIN(NCL + 1), PFQ(NCL + 1), PLANK(NFO,NCL)
3367            REAL*8 PDIN(NFO,NCL + 1), PITE(NFO,NCL), PZIN(NFO,NCL)
3368            REAL*8 PAB(NCL)
3369            REAL*8 Q(NANO,NFO,NCL)
3370            REAL*8 SPH, SERC, SPR
3371            REAL*8 SIGM(NFO,NCL), QR1S(NCL + 1)
3372            REAL*8 SOLU(NCL + 1), SPRB
3373            REAL*8 S(NFO,NCL), SUM1, SUM2, QRFQ(NCL), QRZQ(NCL)
3374            REAL*8 SINT(NFO,NCL + 1)
3375            REAL*8 TTIME, TOU, TERR, TELB
3376            REAL*8 TRNFVR(NCL), TEMP(NCL)
3377            REAL*8 UFL
3378            REAL*8 WP(NANO)
3379            REAL*8 ZLP(NANO), ZINT(NFO,NCL), ZQ(NFO,NCL), DIER
3380
3381            COMMON /R01/ ALFA, AC, ATMASS, DAF, ATEM
3382            COMMON /R02/ ABC, AB, AO
3383            COMMON /R03/ BETA, BO
3384            COMMON /R04/ CV, CW, CH
3385            COMMON /R05/ DL, DINT, PRNTM
3386            COMMON /R06/ DIST, DTIME, DSPR
3387            COMMON /R07/ ETA
3388            COMMON /R07I/ FINT, FINL, FINR
3389            COMMON /R08/ FR, FQ
3390            COMMON /R09/ HELIM
3391            COMMON /R10/ INLB, INRB, ITEL, IERED, IERR
3392            COMMON /R11/ INTB, IINT, IZIN
```

```
      COMMON /R12/ ITRB, ITER
      COMMON /R13/ L, LPL, LOWLIM
      COMMON /R14/ MAXT
      COMMON /R15/ NATE, NINT
      COMMON /R16/ NFFT, NDIN, NZIN
      COMMON /R17/ PMAC, PINT, PRTIME
      COMMON /R18/ POIN, PFOI, PLANK
      COMMON /R181/ PDIN, PITE, PZIN
      COMMON /R182/ PAB
      COMMON /R19/ Q
      COMMON /R20/ SPH, SIRC, SPR
      COMMON /R21/ SIOM, ORSI
      COMMON /R22/ SOLU, SPRB
      COMMON /R23/ S, SUM1, SUM2, ORFQ, GRZQ
      COMMON /R231/ SINT
      COMMON /R24/ TTIME, TOU, TERR, TELB
      COMMON /R25/ TRNFVR, TEMP
      COMMON /R26/ UPL
      COMMON /R27/ WF
      COMMON /R28/ ZLP, ZINT, ZQ, DIER

      INTEGER IFL, NTR
      EXTERNAL FFLNK, F2, F3

      INTEGER NRN, NCODE, NCOUNT, PRNT
      COMMON /RDC/ NRN, NCODE, NCOUNT, PRNT

      REAL*8 ABS(NCL)
      REAL*8 DD, DMIN
      REAL*8 EE, ENERGL(-NFO), ENERGR(NFO)
      REAL*8 INBR(NCL)
      REAL*8 JUNK(NFO,NCL), JUNK2(NFO,NCL), SUMINK(NCL)
      REAL*8 PV, POVER(NFO,NCL), PLSON(NFO,NCL)
      REAL*8 RESPLN
      REAL*8 SPLAN(NCL), SUMCH(NCL)
      REAL*8 TMIN
      REAL*8 XA, XSA(NFO,NCL), XAA
      REAL*8 ZFAC, ZFAC1, ZTMAX
      REAL*8 NR(151)
      REAL*8 RSPH(150)
      COMMON /RCV/ RSPH
      IMPLICIT REAL*8(A - H,O - Z)
C****  beginning of modcon common blocks
C
CL       C2.1  HYDRODYNAMICS
C  VERSION 1A    1/8/73    JPC     CULHAM
      COMMON /COMHYD/ DM, P3, PIN1, R1, R3, R5, RHO1, RHO3, RHO5,
     1    RHOIN1, RHOR, RIN1, TIME, U2, U4, UEDGE, V1, V3, V5
      DIMENSION DM(151), P3(151), R1(151), R3(151), R5(151), RHO1(151),
     1    RHO3(151), RHO5(151), U2(151), U4(151), V1(151),
     2    V3(151), V5(151)
C
CL       C2.2  THERMODYNAMICS
C  VERSION 1A    1/8/73    JPC     CULHAM
      COMMON /COMTH/ DDROE1, DDROE3, DDRO1, DDRO3, DDTE1, DDTE3,
     1    DDTI1, DDTI3, GAMMAE, GAMMAI, KAPPAE, KAPPAI, PE1, PE3,
     2    PI1, PI3, TE1, TE3, TEIN1, TI1, TI3, TIN1
      REAL*8 KAPPAE, KAPPAI
      DIMENSION DDROE1(151), DDROE3(151), DDRO1(151), DDRO3(151),
     1    DDTE1(151), DDTE3(151), DDTI1(151), DDTI3(151),
     2    KAPPAE(151), KAPPAI(151), PE1(151), PE3(151), PI1(151),
     3    PI3(151), TE1(151), TE3(151), TI1(151), TI3(151)
C
CL       C2.3  IONS AND ELECTRONS
C  VERSION 1A    1/8/73    JPC     CULHAM
      REAL*8 LC, MEFF, NE, NI
      COMMON /COMDE/ BREMS1, BREMS3, DEOEN, DEOMAX, DEOMIN, EFFZ,
     1    EDCH2, LC, MEFF, NI, NE, OMEGA1, PZ1, PZ3, PZSQ1, PZSQ3,
     2    DDZ1, DDZ3, PEDASH, PMASS
      DIMENSION BREMS1(151), BREMS3(151), DEOEN(151), EFFZ(151),
     1    EDCH2(151), LC(151), MEFF(151), NE(151), NI(151),
     2    PZ1(151), PZ3(151), PZSQ1(151), PZSQ3(151), DDZ1(151),
     3    DDZ3(151), PEDASH(151), OMEGA1(151)
C
CL       C2.4  LASER VARIABLES
C  VERSION 1A    1/8/73    JPC     CULHAM
C     REAL*8       LAMDA1,   LASER1, NSCRIT
      COMMON /COMLAS/ ALPHA1, ELAS1, LAMDA1, LASER1, PLAS1, RABS1,
     1    RSCRI1, XL1, XL3, NSCRI1, PRACL8, NABS1
      DIMENSION ALPHA1(151), LASER1(100), XL1(151), XL3(151)
C
CL       C2.5  THERMONUCLEAR REACTIONS
C  VERSION 1A    1/8/73    JPC     CULHAM
      COMMON /COMFUS/ DEUTER, F1D, F3D, F1H, F3H, F1HE3, F3HE3, F1HE4,
     1    F3HE4, F1NEU, F3NEU, F1NTRL, F3NTRL, F1T, F3T, F1X, F3X,
     2    HELEU3, HELRU4, HYDROG, NETRAL, NTRLMB, PNEUT1, PNEUT3,
     3    R1DD, R3DD, R1DHE3, R3DHE3, R1DT, R3DT, RNEUT1, RNEUT3,
     4    TINUCL, TOTNEU, TRITIU, XMASS, XTRA, XZ, YE1, YE3, YI1,
     5    YD, YHELD, XTRA1, XTRA2, XTRA3, XZ1, XZ2, XZ3, XMASS1,
     6    XMASS2, XMASS3, XTRA4, XZ4, XMASS4, F1X1, F1X2, F1X3, F3X1,
     7    F3X2, F3X3, F1X4, F3X4
      REAL*8 NETRAL, NTELMB
      DIMENSION F1D(151), F3D(151), F1H(151), F3H(151), F1HE3(151),
     1    F3HE3(151), F1HE4(151), F3HE4(151), F1NEU(151),
     2    F3NEU(151), F1NTRL(151), F3NTRL(151), F1T(151),
     3    F3T(151), F1X(151), F3X(151), F1X1(151), F1X2(151),
     4    F1X3(151), F1X4(151), F3X1(151), F3X2(151), F3X3(151),
     5    F3X4(151), R1DD(151), R3DD(151), R1DHE3(151),
     6    R3DHE3(151), R1DT(151), R3DT(151), YE1(151), YE3(151),
     7    YI1(151), YD(151)
C
CL       C2.8 NON-LTE DATA FOR AVRO-Z,RADIATIVE COOLING ETC...
C  VERSION JUNE 1986 Y.T. LEE
      COMMON /LEEXLY/ HNUEDO(64), DTEMP(19), DDENS(22), ENION(19,22),
     1    TBLZ(19,22), TBLZSQ(19,22), POWER(19,22,64),
     2    SIOMA(19,22,64), HNUMIN, HNUMAX, ZATOM, NT, NR, NOHION,
     3    NOLOW, NORMAX, NTMAX
C
C-----------------------------------------------------------------
CL  C0.0  AUXILIARY X-RAY TRANSPORT ARRAYS FOR USE WITH LEE'S TABLES
C
      REAL*8 NIB
      COMMON /LEEXR2/ RADTL, RADTR, PPL1, PPR1, DT2B, PRDLL1(64),
     1    PRDLR1(64), PRADLL(64), PRADLR(64), RADLL(64), RADLR(64),
     2    TE1B(151), NIB(151), REDOEB
C-----------------------------------------------------------------
CL       C3.2  MESH AND NUMERICAL METHODS
C  VERSION 1A    1/8/73    JPC     CULHAM
      COMMON /COMNUM/ AE, AI, BE, BI, CE, CI, DE, DI, E, F, OE, OI, Q2,
     1    Q4, TEITE, TITE, UITE, MESH, NJ, NJM1, NJP1, NL, NLM1,
     2    NLP1
      DIMENSION AE(151), AI(151), BE(151), BI(151), CE(151), CI(151),
     1    DE(151), DI(151), E(151), F(151), OE(151), OI(151),
     2    Q2(151), Q4(151), TEITE(151), TITE(151), UITE(151)
C
CL       C2.9 RADIATION REABSORPTION
C  VERSION JUNE 1984, D. SALZMANN
      COMMON /COMABS/ YONS(151), DO(20,15)
C
CL       C2.7  PHYSICS CONTROL
C  VERSION 1A    1/8/73    JPC     CULHAM
      COMMON /COMCON/ FMIN, RHOMIN, TEMIN, TIMIN, UMIN, MSTEP, NCASE,
     1    NOBOM, MLBRMB, MLBCON, MLFUSE, MLICON, MLX, NLABS, NLBRMS,
     2    NLBURN, NLCRI1, NLDEPO, NLECON, NLFUSE, NLICON, NLMOVE,
     3    NLPPE, NLPP1, NLX
      LOGICAL MLBRMB, MLBCON, MLFUSE, MLICON, MLX, NLABS, NLBRMS,
     1    NLBURN, NLCRI1, NLDEPO, NLECON, NLFUSE, NLICON, NLMOVE,
     2    NLPPE, NLPP1, NLX
C
CL       C3.1  NUMERICAL CONTROL PARAMETERS
C  VERSION 1A    1/8/73    JPC     CULHAM
      COMMON /COMNC/ AK0, AK1, AK2, AK3, AK4, AK5, BNEUM, DELTAT, DT2,
     1    DT3, DT4, DTEMAX, DTIMAX, DTMAX, DTMIN, DUMAX, RDT2, RDT3,
     2    RDT4, NCELDT, NCONDT, NIT, NITMAX, BREAK, NLGOON, NLITE
      LOGICAL BREAK, NLGOON, NLITE
C
CL       C4.1  ADMINISTRATIVE VARIABLES
C  VERSION 1A    1/8/73    JPC     CULHAM
      COMMON /COMADM/ PIQ, TSTOP, MAXDIM, MAXRUN, NDUMP, NREP, NLDUMP,
     1    NLEMP
      LOGICAL NLDUMP, NLEMP
      DIMENSION PIQ(100)
C
      COMMON /COMUT1/ ZWMAR1(151), ZWMAR2(151), ZWMAR3(151),
     1    ZWMAR4(151), ZWMAR5(151), ZWMAR6(151), ZWMAR7(151),
     2    ZWMAR8(151), ZWMAR9(151), ZWMA10(151), ZWMA11(151),
     3    ZWMA12(151), ZWMA13(151), ZWMA14(151), ZWMA15(151),
     4    ZWMA16(151)
C-----------------------------------------------------------------
C  COMMON/SHELL/RSHELL(11),NSHELL(11),QSHELL(11),NBMAX
      COMMON /SHELL/ RSHELL, QSHELL, NSHELL, NBMAX
      DIMENSION RSHELL(11), QSHELL(11), NSHELL(11)
      EQUIVALENCE (PIQ(63),ZPLAS), (PIQ(62),ROPLAS), (PIQ(61),DRPLAS),
     1    (PIQ(39),STATE), (PIQ(58),RAHA), (PIQ(56),PONDF),
     2    (PIQ(37),RHOT), (PIQ(37),GAUSS), (PIQ(52),ANABS),
     3    (PIQ(22),FTHOT), (PIQ(21),FHOT), (PIQ(14),FNE),
     4    (PIQ(13),ZOLAS), (PIQ(12),ROOLAS), (PIQ(11),DROLAS),
     5    (PIQ(10),PLIMIT), (RHOIN,RHOGAS), (LASER1(1),TON),
     6    (LASER1(2),FMULT), (LASER1(3),ANPULE), (LASER1(4),
     7    PLENTH), (LASER1(5),TOFF), (LASER1(6),PMAX),
     8    (PIQ(60),SIMULT), (PIQ(64),OUTAMI), (PIQ(66),DTPRNT)
      EQUIVALENCE (PIQ(67),NELEDO)
C-----------------------------------------------------------------
CL       C1.1.  BASIC SYSTEM PARAMETERS
C  VERSION 2B      14.8.73   KVR/MRH     CULHAM
C-----------------------------------------------------------------
CL       C1.1.  BASIC SYSTEM PARAMETERS
C  VERSION 2B      14.8.73   KVR/MRH     CULHAM
      COMMON /COMBAS/ ALTIME, CPTIME, NLEDGE, NLEND, NLRES, NONLIN,
     1    NOUT, NPRINT, NREAD, NRJEC, NRESUM, NSTEP, STIME, LABEL1,
     2    LABEL2, LABEL3, LABEL4, LABEL5, LABEL6, LABEL7, LABEL8,
     3    NDIARY, NIN, NPUNCH, NRUN
      LOGICAL NLEND, NLRES
      DIMENSION LABEL1(12), LABEL2(12), LABEL3(12), LABEL4(12),
     1    LABEL5(12), LABEL6(12), LABEL7(12), LABEL8(12)

C****  end of modcon common blocks
   IF (MDT .EQ. 0) THEN
C**** initialization of the variables
C**** nult is set to 1 once this subroutine returns to main subroutine
      DATA NTR /0/, AN /6.022E24/, EPS, EPS1, EPS2 /1.E-9, 1.E-3, 1.E-
     1    1/
      IF (NTR .EQ. 0) THEN
        NTR = 1
        NC = NL
        NCP1 = NC + 1
        NCM1 = NC - 1
        NO = NOHION - NOLOW
        TMIN = 0.5 * (10.0**DTEMP(1))
        DMIN = 10.0 ** DDENS(1)
        IZP1 = ZATOM + 1.
        IF (TIME .EQ. 0.0) TI2D=
        DT2B = DT2
        DO 10 K = 1, NC
          NIB(K) = NI(K)
          TE1B(K) = TE1(K)
   10     CONTINUE
        REDOEB = R1(NCP1)
        RADTL = 0.0
        RADTR = 0.0
        PPL1 = 0.0
        PPR1 = 0.0
```

```
3605              DO 20 J = 1, NG + 1
3606                PRADLL(J) = 0.0
3607                PRADLR(J) = 0.0
3608                PRDLL1(J) = 0.0
3609                PRDLR1(J) = 0.0
3610                RADLL(J) = 0.0
3611                RADLR(J) = 0.0
3612             20   CONTINUE
3613              END IF
3614            END IF
3615            DTIME = DT2
3616            ATMASS = XMASS
3617            TOU = 1 / (SP*DTIME)
3618            NITT = NIT
3619            IF (NIT .NE. 1) RETURN
3620          C**** extrapolate ta3 using the slope of the previous step
3621            DO 30 K = 1, NC
3622              Z1 = (TE1(K) - TE1B(K)) * DT2 / DT2B
3623              IF (ABS(Z1) .GT. 0.5*TE3(K)) Z1 = 0.0
3624              TE3(K) = TE1(K) + Z1
3625              NB0(K) = NB(K)
3626              Z1 = (NB(K) - NB0(K)) * DT2 / DT2B
3627              IF (ABS(Z1) .GT. 0.5*NB(K)) Z1 = 0.0
3628              NB(K) = NB(K) + Z1
3629             30   CONTINUE
3630              Z1 = (R1(NCP1) - REDGEB) * DT2 / DT2B
3631              IF (ABS(Z1) .GT. 0.5*R1(NCP1)) Z1 = 0.0
3632              REDGEB = R1(NCP1) + Z1
3633              DO 40 K = 1, NC
3634                BREMB3(K) = 0.0
3635             40   CONTINUE
3636              DO 50 J = 1, NG + 1
3637                PRADLL(J) = 0.0
3638                PRADLR(J) = 0.0
3639             50   CONTINUE
3640              ZTMAX = TE3(NABS1)
3641              DO 60 K = NABS1, NC
3642                ZTMAX = DMAX1(ZTMAX,TE3(K))
3643             60   CONTINUE
3644              IF (ZTMAX .LE. TMIN) THEN
3645          C**** skip radiation code
3646                RTEON = .FALSE.
3647                WRITE (6,70) NCOUNT, TIT, TIME
3648             70   FORMAT ('radiation code skipped due to low temp in rte.f',
3649              1       2(1X,I4), 1X, 1PE11.4)
3650                GO TO 670
3651              ELSE
3652                RTEON = .TRUE.
3653              END IF
3654              DO 80 K = 1, NC
3655                ATEM4(K) = TE3(K)
3656          C**** rajh is obtained from EOS subroutine in MEDUSA
3657                CV(K) = RMPH(K) * RHO3(K) / 10.0
3658                DIST(K) = R1(K)
3659                DL(K) = ABS(R1(K + 1) - R1(K))
3660             80   CONTINUE
3661          C**** define the frequency groups
3662              DO 90 JJ = NGLOW, NGHIGH
3663                J = JJ - NGLOW + 1
3664                FR(J) = HNUEDG(JJ)
3665             90   CONTINUE
3666          C**** find the power and x-sectional area at given temperature
3667          C**** and density by interpolation. (power='W/m**2, x-area='m**2 and
3668          C**** abs coef='1/m)
3669              DO 120 K = 1, NC
3670                IF (TE3(K) .GE. TMIN) THEN
3671                  DO 100 JJ = NGLOW, NGHIGH
3672                    J = JJ - NGLOW + 1
3673                    XAA = CKIMA(DLOG10(0.5*(HNUEDG(J) + HNUEDG(J + 1))),ZATOM)
3674              1       * ATMASS / AN
3675          C**** zfac1 = 0.0 if ta3 < tmin, otherwise zfac1 = 1.0
3676                    ZFAC1 = DMAX1 (0.0D0,DMIN1(1.0D0,(TE3(K) - TMIN)/TMIN))
3677          C**** zfac = 0.0 if ta3 < tmin, otherwise zfac == 1.0
3678                    ZFAC = ZFAC1 * DMIN1(1.0D0,NB(K)/DMIN)
3679                    CALL DINTRP(DLOG10(TE3(K)), DLOG10(NB(K)), SIGMA(1,1,JJ),
3680              1         XA, IFL)
3681                    XSA(JJ,K) = (1.0 - ZFAC1) * XAA + ZFAC1 * 10.0 ** XA
3682                    XSA(JJ,K) = 10.0 ** XA
3683                    ABC(JJ,K) = NB(K) * XSA(JJ,K)
3684          CC          ABC(JJ,K) = (RHO3(K)*AN*XSA(JJ,K)) / ATMASS
3685                    CALL INTRP(POWER3(1,1,JJ), PV)
3686                    PLANK(JJ,K) = ZFAC * 10.0 ** PV * NB(K) * DL(K) / (4*PI)
3687          CC          PLANK(JJ,K) = ZFAC*10.0**PV/(4*PI*XSA(JJ,K))
3688                  100   CONTINUE
3689          C**** rtabbm
3690                ELSE
3691                  DO 110 JJ = NGLOW, NGHIGH
3692                    J = JJ - NGLOW + 1
3693                    XAA = CKIMA(DLOG10(0.5*(HNUEDG(J) + HNUEDG(J + 1))),ZATOM)
3694              1       * ATMASS / AN
3695                    ZFAC1 = DMAX1 (0.0D0,DMIN1(1.0D0,(TE3(K) - TMIN)/TMIN))
3696                    ZFAC = ZFAC1 * DMIN1(1.0D0,NB(K)/10.0**DOUBNK(1))
3697                    CALL DINTRP(DLOG10(TE3(K)), DLOG10(NB(K)), SIGMA(1,1,JJ),
3698              1         XA, IFL)
3699                    XSA(JJ,K) = (1.0 - ZFAC1) * XAA + ZFAC1 * 10.0 ** XA
3700          C           XSA(JJ,K) = XAA
3701                    ABC(JJ,K) = NB(K) * XSA(JJ,K)
3702          CC          ABC(JJ,K) = (RHO3(K)*AN*XSA(JJ,K)) / ATMASS
3703                    DD = HNUEDG(JJ) * 11604.0 / TE3(K)
3704                    EE = HNUEDG(JJ + 1) * 11604.0 / TE3(K)
3705                    IF (DD .GT. LOWLIM) THEN
3706                      DD = LOWLIM
3707                    END IF
3708                    IF (EE .GT. HILIM) THEN
3709                      EE = HILIM
3710                    END IF
3711                    CALL ROMB(FPLNK, DD, EE, RESPLN)
3712                    PLANK(JJ,K) = (2*PK/SP**2) * ((BK*TE3(K)/PK)**4) * RESPLN
3713                  110   CONTINUE
3714                END IF
3715                120   CONTINUE
3716              DO 150 K = 1, NC
3717                AB(K) = 0.0
3718                DO 140 J = 1, NG
3719                  ZINT(J,K) = 0.0
3720                  DO 130 I = 1, NA
3721                    PINT(I,J,K) = PLANK(J,K)
3722                    IINT(I,J,K) = PLANK(J,K)
3723                    ZINT(J,K) = ZINT(J,K) + IINT(I,J,K) * WF(I)
3724                  130   CONTINUE
3725                  IZIN(J,K) = ZINT(J,K)
3726                  AB(K) = AB(K) + ABC(J,K) * ZINT(J,K)
3727                140   CONTINUE
3728              150   CONTINUE
3729                IF (PRES .GE. 5 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
3730               1    THEN
3731                  WRITE (8,160) (K,DL(K),CV(K),ATEM4(K)/11604,IERED(K),K=1,NC)
3732                160   FORMAT (2('k',I2,1X,'dl=',1PE10.3,1X,'cv=',1PE10.3,1X,'temp=',
3733               1       1PE10.3,1X,'Ue=',1PE10.3,1X))
3734                  WRITE (8,*)'freq group limits in tables ', DTIME
3735                  WRITE (8,170) (J,FR(J),J=1,NG + 1)
3736                170   FORMAT (8('g',I2,1X,F11.4,1X))
3737                  WRITE (8,*)'i j k iint in tables'
3738                  WRITE (8,180) (((I,J,K,IINT(I,J,K),K=1,NC),J=1,NG),I=1,NA)
3739                180   FORMAT (6('I',I2,1X,'J',I2,1X,'k',I2,1X,1PE10.3,1X))
3740                  WRITE (8,*)'j k zint in tables '
3741                  WRITE (8,190) (J,K,ZINT(J,K),K=1,NC),J=1,NG)
3742                190   FORMAT (8(I2,1X,I2,1X,1PE10.3,1X))
3743                END IF
3744                DO 210 K = 1, NC
3745                  ABB(K) = 0.0
3746                  SPLAN(K) = 0.0
3747                  DO 200 J = 1, NG
3748                    ABB(K) = ABB(K) + ABC(J,K) * PLANK(J,K)
3749                    SPLAN(K) = SPLAN(K) + PLANK(J,K)
3750                200   CONTINUE
3751                210   CONTINUE
3752              DO 230 K = 1, NC
3753                SUMCHI(K) = 0.0
3754                DO 220 J = 1, NG
3755                  CHI(J,K) = ABC(J,K) * PLANK(J,K) / ABB(K)
3756                  SUMCHI(K) = SUMCHI(K) + CHI(J,K)
3757                  IERED(K) = 4 * PI * SPLAN(K) / SP
3758                220   CONTINUE
3759              230   CONTINUE
3760                IF (PRES .GE. 1) THEN
3761                  WRITE (8,240) TE3(1), DDTE3(1), DDTI3(1), RHO3(1), CV(1),
3762               1    RSPH(1), DM(1), DL(1), ATMASS, VX(1)
3763                240   FORMAT ('U the dti ro cv qp dm dl stm v=' ', 10(1X,1PE10.3))
3764                END IF
3765                IF (PRES .GE. 21) THEN
3766                  WRITE (8,*)'sumchi in tables '
3767                  WRITE (8,250) (K,SUMCHI(K),K=1,NC)
3768                250   FORMAT (8(I2,1X,1PE11.4,1X))
3769                END IF
3770                DO 260 K = 1, NC
3771                  BETA(K) = 4 * RK * (TE3(K)**3) / CV(K)
3772                  PMAC(K) = ABB(K) / SPLAN(K)
3773                  ALFA(K) = 1 / (PMAC(K)*BETA(K))
3774                  TENFVR(K) = SP * DTIME / DL(K)
3775                  ETA(K) = 1 / (1 + ALFA(K)*TOU)
3776                260   CONTINUE
3777                  SIRC = 0.0
3778                  DO 270 K = 1, NC
3779                    SIRC = SIRC + ETA(K)
3780                270   CONTINUE
3781                  SIRC = SIRC / NC
3782                  DO 300 J = 1, NG
3783                    DO 290 K = 1, NC
3784                      FQ(J,K) = 0.0
3785                      DO 280 I = 1, NA
3786                        Q(J,K) = CHI(J,K) * IERED(K) * ETA(K) / (2*DTIME*BETA(K)
3787               1        ) + TOU * IINT(I,J,K)
3788                        FQ(J,K) = FQ(J,K) + IINT(I,J,K) * WF(I) * ZLP(I)
3789                280     CONTINUE
3790                      SIGMA(J,K) = (ABC(J,K) + TOU) * DL(K)
3791                      ZQ(J,K) = CHI(J,K) * IERED(K) * ETA(K) / (DTIME*BETA(K)) +
3792               1      TOU * IZIN(J,K)
3793                290   CONTINUE
3794                300   CONTINUE
3795                  IF (PRES .GE. 5 .AND. TOIT .GE. DBXL .AND. TOIT .LE. DBXU)
3796               1    THEN
3797                    WRITE (8,*)'sum of chis and sbbchi in tables '
3798                    WRITE (8,310) (K,SUMCHI(K),SUMNK(K),K=1,NC)
3799                310   FORMAT (5(I2,1X,2(1PE11.4,1X)))
3800                    WRITE (8,*)'j k chi sbc plank in tables '
3801                    WRITE (8,320) ((J,K,CHI(J,K),ABC(J,K),PLANK(J,K),J=1,NG),K=1,
3802               1    NC)
3803                320   FORMAT (3(I2,1X,I2,1X,3(1PE10.3,1X)))
3804                    WRITE (8,*)' i j k q in tables '
3805                    WRITE (8,330) (((J,K,Q(J,K),K=1,NC),J=1,NG),I=1,NA)
3806                330   FORMAT (6(I2,1X,I2,1X,I2,1X,1PE10.3,1X))
3807                    PAUSE
3808                  END IF
3809                  DO 350 K = 1, NC
3810                    GRZQ(K) = 0.0
3811                    GRFQ(K) = 0.0
3812                    DO 340 J = 1, NG
3813                      GRZQ(K) = GRZQ(K) + ZQ(J,K)
3814                      GRFQ(K) = GRFQ(K) + FQ(J,K) / SIGMA(J,K)
3815                340   CONTINUE
3816                350   CONTINUE
```

```
      DO 360 J = 1, NG
        INLB(J) = 0.0
        INRB(J) = 0.0
  360 CONTINUE
      IF (NPFC .EQ. 0) THEN
        DO 370 K = 1, NC
          TRNFVR(K) = 0.5
  370   CONTINUE
        TRNFV = (SP*DTIME) / DL(1)
      ELSE IF (NPFC .EQ. 1) THEN
        DO 380 K = 1, NC
          TRNFVR(K) = 2.0
  380   CONTINUE
        TRNFV = (SP*DTIME) / DL(1)
      ELSE IF (NPFC .EQ. 2) THEN
        DO 390 K = 1, NC
          TRNFVR(K) = (SP*DTIME) / DL(K)
  390   CONTINUE
      END IF
      DO 410 K = 1, NC
        INBR(K) = 0.0
        DO 400 J = 1, NG
          INBR(K) = INBR(K) + 4 * PI * PLANK(J,K) / D40(K)
  400   CONTINUE
  410 CONTINUE
      RETURN
      END IF
      IF (PRES .GE. 4) THEN
       WRITE (8,*)'j k iint nint nint/iint in tables'
       WRITE (8,420) (((J,K,IINT(J,J,K),NINT(J,J,K),NINT(J,J,K)/IINT(
     1 J,J,K),J=1,NA),J=1,NG),K=NC - 5,NC)
  420  FORMAT (3(I*,I2,1X,)/,I2,1X,W.I2,1X,3(1PE10.3,1X)))
       END IF
C***** brems - power emitted per unit mass  watts/Kg
      DO 450 K = 1, NCP1
        DO 440 J = 1, NG
          DINT(J,K) = 0.0
          DO 430 I = 1, NA
            DINT(J,K) = DINT(J,K) + INTB(J,J,K) * WP(I) * ZLP(I)
  430     CONTINUE
  440   CONTINUE
  450 CONTINUE
      DO 480 K = 1, NC
        BREMS3(K) = 0.0
        DO 470 J = 1, NG
          DO 460 I = 1, NA
            BREMS3(K) = BREMS3(K) + (2*PI/DM(K)) * (INTB(J,J,K + 1) -
     1      INTB(J,J,K)) * WP(I)
  460     CONTINUE
  470   CONTINUE
  480 CONTINUE
C***** flux emitted from right end of the plasma watts/m^2
      DO 510 J = 1, NG
        PRADLR(J) = 0.0
        DO 500 K = NC, NC
          DO 490 I = 1, NAD2
            PRADLR(J) = PRADLR(J) + (2*PI) * INTB(J,J,K + 1) * WP(I) *
     1      ZLP(I)
  490     CONTINUE
  500   CONTINUE
        FLUXR = FLUXR + PRADLR(J)
  510 CONTINUE
C***** flux emitted from left end of the plasma watts/m^2
      DO 540 J = 1, NG
        PRADLL(J) = 0.0
        DO 530 K = 1, 1
          DO 520 I = NAD2, NA
            PRADLL(J) = PRADLL(J) + (2*PI) * INTB(J,J,K) * WP(I) * AB8(
     1      ZLP(I))
  520     CONTINUE
  530   CONTINUE
        FLUXL = FLUXL + PRADLL(J)
  540 CONTINUE
      DUMTIME = DUMTIME + TIME
      IF (DUMTIME .GE. DTPRNT/2.5) THEN
        DUMTIME = 0.0
        WRITE (7,550) TIME, FLUXL, FLUXR
  550   FORMAT ('fluxl & fluxr in rte.f = ', 3(1PE11.4,1X))
        DO 580 J = 1, NG
          ENERGL(J) = 0.0
          ENERGR(J) = 0.0
          DO 570 I = 1, NA
            DO 560 K = NAB81, NAB81
              ENERGL(J) = ENERGL(J) + NINT(J,J,K - 2)
              ENERGR(J) = ENERGR(J) + NINT(J,J,K + 2)
  560       CONTINUE
  570     CONTINUE
  580   CONTINUE
        WRITE (11,590) (HNUEDG(J),ENERGL(J),ENERGR(J),J=1,NG)
  590   FORMAT (3(1PE12.5,1X))
        END IF
        IF (PRES .GE. 2) THEN
          CALL TEMPER
          WRITE (6,*)'after solving rte te3 te1 rate brems inibr in rte.f'
          WRITE (6,600) (K,TE1(K),TE3(K),NATE(K),BREMS3(K),INBR(K),K=1,
     1    NC)
  600     FORMAT (2(I2,1X,5(1PE10.3,1X)))
          IF (PRES .GE. 2) THEN
            DO 620 K = 1, NC
              DO 610 JJ = NGLOW, NGHIGH
                J = JJ - NGLOW + 1
                DD = HNUEDG(JJ) * 11604.0 / NATE(K)
                EE = HNUEDG(JJ + 1) * 11604.0 / NATE(K)
                IF (DD .GT. LOWLIM) THEN
                  DD = LOWLIM
                END IF
```



```
                IF (EE .GT. HILIM) THEN
                  EE = HILIM
                END IF
                CALL ROMB(FPLNK, DD, EE, RESPLN)
C               WRITE (6,*)'resl ', RESPLN
                PLNKN(J,K) = (2/(SP**2)) * (NATE(K)**4) * (BK*TCF) *
     1          RESPLN / (A0**3)
  610         CONTINUE
  620       CONTINUE
            WRITE (8,*)'plankian before after solving rte'
            WRITE (8,630) ((J,K,IZINJ(J,K),PLNKN(J,K),K=1,NC),J=1,NG)
  630       FORMAT (4(2(I2,1X),2(1PE10.3,1X)))
          END IF
          PAUSE
        END IF
        NPR = NPR + 1
        IF (NPR .GE. 100) THEN
          WRITE (6,640) TIME, DTIME, TRNACC, DIFACC, TOIT, TIIT, TIT, SPR
  640     FORMAT (1X,'t dt tr df tot tot tit spr=', 2(1PE10.3,1X),
     1      2(I1,1X), 2(I7,1X), I6, 1X, 1PE9.2)
          NPR = 0
        END IF
  650 CONTINUE
C***** return original values
      DT2B = DT2
      DO 660 K = 1, NC
        NEK(K) = NE0(K)
        NI(K) = NI0(K)
        TE1B(K) = TE1(K)
        TE3(K) = TE1(K)
  660 CONTINUE
      REDGEB = R1(NCP1)
      RETURN
      END
```